

Fluctuation energies in quantum cosmology

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Abstract

Quantum fluctuations or other moments of a state contribute to energy expectation values and can imply interesting physical effects. In quantum cosmology, they turn out to be important for a discussion of density bounds and instabilities of initial-value problems in the presence of signature change in loop-quantized models. This article provides an effective description of these issues, accompanied by a comparison with existing numerical results and an extension to squeezed states. The comparison confirms that canonical effective methods are well-suited for computations of properties of physical states. As a side product, an example is found for a simple state in which quantum fluctuations can cancel holonomy modifications of loop quantum cosmology.

1 Introduction

Fluctuation energies are well-known from the main example of the zero-point energy, an energy contribution that depends on quantum fluctuations and is evaluated for the ground state. Heuristically, the ground state has a non-vanishing energy, in contrast to the classical theory, because the uncertainty principle does not allow both the position and the momentum fluctuation to be zero. While expectation values of position and momentum can minimize the classical energy function, quantum fluctuations provide an additional zero-point energy. One can see the relationship to quantum fluctuations clearly by writing the energy expectation value of the harmonic oscillator, in an arbitrary state, as

$$\langle \hat{E} \rangle = \frac{\langle \hat{p} \rangle^2}{2m} + \frac{1}{2}m\omega^2 \langle \hat{x} \rangle^2 + \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2 (\Delta x)^2. \quad (1)$$

In a stationary state, one has $\langle \hat{x} \rangle = 0 = \langle \hat{p} \rangle$, and only the fluctuation terms remain. If one inserts the ground-state values $(\Delta x)^2 = \hbar/(2m\omega)$ and $(\Delta p)^2 = \frac{1}{2}m\omega\hbar$, one obtains the zero-point energy $\frac{1}{2}\hbar\omega$.

Although such fluctuation terms can contribute to any state of a system in quantum mechanics, they are usually not considered significant for semiclassical states. In this article, we discuss the analogous notion for quantum cosmology. The situation is then rather different because the systems considered in this field do not give rise to a natural ground

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state. The more-general notion of fluctuation energies is therefore preferred compared to zero-point energies. Quantum fluctuations (or other moments of a state) may not seem to contribute a significant amount compared with the total matter energy contained in the universe. However, several quantum-geometry effects have been suggested for quantizations of space-time. Some of them, for instance in loop quantum cosmology, imply corrections to the classical Friedmann equation which are able to cancel the classical matter energy in certain regimes. If a fluctuation energy is left after the cancellation, it may have some influence on the dynamics of a universe model.

The main example for such a cancellation effect is the “bounce” scenario proposed in loop quantum cosmology, based on the modified (spatially flat) Friedmann equation

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho \left(1 - \frac{\rho}{\rho_{\text{QG}}}\right) \quad (2)$$

with a quantum-gravity parameter ρ_{QG} which one can think of as being close to the Planck density [1, 2]. (This equation has been derived in a reliable way for models sourced by a free, massless scalar [3].) Near $\rho \sim \rho_{\text{QG}}$, quantum-geometry corrections may cancel the classical term of the matter energy density. A solution with $\dot{a} = 0$ at one time then becomes possible, leading to a turn-around of the scale factor at high density. If there is a fluctuation-dependent contribution to (2), viewed as an effective equation of quantum cosmology, it may become significant near $\rho \sim \rho_{\text{QG}}$ and might change the dynamics as well as the density realized at the bounce.

As it turned out, loop quantum cosmology is not viable as a stand-alone universe model. The modification seen in the isotropic background equation (2) also affects equations for inhomogeneous fields. As a consequence, one can show that the underlying space-time structure is drastically modified compared to the classical one [4, 5, 6, 7]. (It remains consistent and anomaly-free, presenting an effective model of quantum space-time.) These effects are visible only when inhomogeneity is included in the equations in a consistent way, paying due attention to covariance and the gauge transformations it is related to. If one were to fix the gauge before considering quantum corrections or to implement other restrictions of the gauge structure, these space-time effects would be missed. Exactly homogeneous minisuperspace models or models in which inhomogeneous modes are added on to the minisuperspace dynamics therefore cannot be considered reliable. (See [8, 9] for detailed discussions.)

The main example for unexpected quantum space-time effects in loop quantum gravity is signature change at high density [10, 11]: Space-time turns into a quantum version of 4-dimensional Euclidean space before the density ρ_{QG} is reached. Accordingly, equations for inhomogeneous fields in this regime are elliptic rather than hyperbolic and do not allow well-posed initial-value problems. There is no causal structure and no deterministic evolution through high density, implying that an interpretation of minisuperspace dynamics as bounce models, according to equations such as (2), is incorrect.

Nevertheless, some properties of background solutions in loop quantum cosmology are of interest for details of the signature-change transition at high density. In this context, we

analyze fluctuation energies contributing to (2). We present two applications in Section 3: An estimate of the severeness of instabilities of an initial-value formulation in the Euclidean phase, and a derivation of several relationships between moments that help to explain some features seen in numerical evolutions of wave functions [12, 13]. An appendix provides more-technical details on expectation values and moments of observables in physical states.

2 States

For a free, massless scalar ϕ with momentum p_ϕ , we have the energy density

$$\rho_{\text{free}} = \frac{1}{2} \frac{p_\phi^2}{a^6}. \quad (3)$$

The classical Friedmann equation of spatially flat models (which is (2) for $\rho_{\text{QG}} \rightarrow \infty$) is equivalent to the Hamiltonian constraint $C = 0$ with the “energy”

$$C = -\frac{3}{8\pi G} a \dot{a}^2 + H_{\text{free}} = -\frac{3}{8\pi G} a \dot{a}^2 + \frac{1}{2} \frac{p_\phi^2}{a^3}. \quad (4)$$

2.1 Dynamical equations

In quantum cosmology, based on Dirac’s formalism to implement constraints, C is quantized to an operator \hat{C} which is to annihilate physical states, $\hat{C}\psi = 0$, as an analog of the classical condition $C = 0$. Acting on states $\psi(a, \phi)$, on which the momentum $p_a = -(3/4\pi G)a\dot{a}$ turns into a derivative operator, we obtain a Wheeler–DeWitt equation [14] of the form

$$\frac{2\pi G \hbar^2}{3} \left(\frac{1}{a} \frac{\partial^2 \psi}{\partial a^2} + \frac{2}{a^2} \frac{\partial \psi}{\partial a} + \frac{1}{4a^3} \psi \right) + \hat{H}_{\text{free}} \psi = 0 \quad (5)$$

with $\hat{H}_{\text{free}} = \frac{1}{2} a^{-3} \hat{p}_\phi^2 = -\frac{1}{2} \hbar^2 a^{-3} \partial^2 / \partial \phi^2$. To be specific, we have chosen one ordering of the non-commuting operators \hat{a} and \hat{p}_a without implying any uniqueness of this choice. As will be shown below, it implies convenient solvability features.

In loop quantum cosmology, the derivative $\partial/\partial a$ is replaced by a difference operator. Not only factor-ordering but also discretization ambiguities then appear, which could be resolved only if one were able to derive cosmological models from the full theory of loop quantum gravity [15, 16, 17]. (But even then, the full theory itself might be subject to ambiguities.) One question is which variable should have an equi-spaced discretization step, a or some function of it. In order to parameterize this ambiguity to some degree, we use a basic canonical pair

$$|Q| := \frac{3a^{2(1-x)}}{8\pi G(1-x)} \quad , \quad P = -a^{2x} \dot{a}. \quad (6)$$

(The variable Q can take both signs, according to the orientation of a spatial triad. Homogeneous variables are defined by spatial integrations and depend on the coordinate volume

of the integration region. For simplicity, we may assume this value to equal one. See [18] for details.) The parameter x is a label for different discretization schemes, so that a quantization of the power $a^{2(1-x)}$ becomes equidistant. This parameter can heuristically be related to the dynamical refinement of spatial lattices underlying states in loop quantum gravity [19, 20]. The most common choice is $x = -1/2$ for equidistant volume $V = 4\pi GQ|_{x=-1/2}$ [2], but it is not unique. The variables (a, p_a) traditionally used in Wheeler–DeWitt quantum cosmology correspond to $x = 1/2$.

Once a value for x has been chosen, the step-size of the corresponding equi-spaced variable Q is determined by another parameter δ , which appears in shift operators $\exp(-i\delta\hat{P})$. One then replaces the classical \dot{a}^2 in the Friedmann equation by a suitable combination of exponentials, such as $\delta^{-2}\sin^2(\delta P)$ times some power of Q , and quantizes them to shift operators. (Sometimes, the first replacement step is done only implicitly.) Instead of the Wheeler–DeWitt equation, the classical constraint turns into a difference equation [21] of the form

$$\begin{aligned} \frac{2\pi G(1-x)^2}{3\delta^2} & \left(|(Q - 2\delta\hbar)(Q - \delta\hbar)|\psi_{Q-2\delta\hbar} - (Q^2 + (Q + \delta\hbar)^2)\psi_Q \right. \\ & \left. + |(Q + 2\delta\hbar)(Q + \delta\hbar)|\psi_{Q+2\delta\hbar} \right) + \frac{1}{2}\hat{p}_\phi^2\psi_Q = 0 \end{aligned} \quad (7)$$

for wave functions $\psi_Q(\phi)$.

In (5) and (7), the ordering we wrote enjoys special properties: It makes the system harmonic and free of quantum back-reaction [3]. We note that this property is a mathematical feature, which by no means implies that the ordering is preferred on physical grounds. However, it is important even for a physical analysis because one can study more-general orderings by perturbation theory around the harmonic model [22, 23, 24] (much as one determines the physics of interacting quantum field theories by perturbation theory around a free theory.) The absence of quantum back-reaction makes it convenient to compute fluctuation energies. Factor orderings other than the one used in (5) or (7) imply additional fluctuation terms which one can compute once the harmonic model is understood.

By solving the Wheeler–DeWitt equation or the difference equation, we obtain “relational” wave functions of the form $\psi(a, \phi)$ or $\psi_Q(\phi)$ instead of time-dependent ones. In this situation, there is no clear meaning of energy eigenvalues where zero-point or fluctuation energies could show up. Nevertheless, expectation values computed for \hat{Q} at fixed ϕ in a solution to the difference equation may be subject to fluctuation-dependent quantum corrections compared to the classical relationship between Q and ϕ . By comparing the behavior of the expectation value with the classical scale factor, these quantum corrections can be interpreted as additional energy contributions in an effective Friedmann equation.

As already mentioned, the ordering matters because re-ordering terms imply additional quantum corrections which depend explicitly on \hbar and can compete with fluctuation terms. Several other popular choices exist in loop quantum cosmology, which follow the same principles of [21], leading to (7), but quantize the relevant operators differently. Of special importance for our purpose will be the treatment of the energy operator provided by the free, massless scalar, a quantization of the classical expression (3). Corresponding operators

have been defined in different ways and analyzed for instance regarding their boundedness properties [25].

When fluctuation terms are interpreted as energy contributions, their precise form depends on how one defines a density expectation value. One may, for instance, define a density operator of the form $\hat{\rho} = \frac{1}{2}\hat{p}_\phi^2\hat{V}^{-2}$ (provided the volume operator \hat{V} is invertible, which is not always the case and sometimes requires additional corrections as per [26]). In some suitable state, this operator then gives rise to an expectation value $\langle\hat{\rho}\rangle$ which one may take as a measure for the energy density. Alternatively, and perhaps more reliably if one considers that canonical quantum gravity provides operators for matter Hamiltonians but not densities, one may define a measure for the energy density as $\langle\hat{E}\rangle/\langle\hat{V}\rangle$ with the energy operator $\hat{E} = \frac{1}{2}\hat{p}_\phi^2\hat{V}^{-1}$.

These two expressions differ by fluctuation terms, as shown by an expansion in moments of the state used. For this purpose, and also for later use, we follow [27] and introduce the moments

$$\Delta(V^a P^b \phi^c p_\phi^d) := \langle(\hat{V} - \langle\hat{V}\rangle)^a (\hat{P} - \langle\hat{P}\rangle)^b (\hat{\phi} - \langle\hat{\phi}\rangle)^c (\hat{p}_\phi - \langle\hat{p}_\phi\rangle)^d\rangle_{\text{Weyl}} \quad (8)$$

using totally symmetric (Weyl) ordering. (More generally, we should refer to our Q instead of V . For the present example, we assume $x = -1/2$, so that the volume, up to a constant factor, is one of our basic variables.) For $a+b+c+d = 2$, we have fluctuations and covariance parameters, such as $\Delta(V^2) = (\Delta V)^2$. Any expression defined as the expectation value of some Weyl-ordered operator $\hat{O} = O(\hat{V}, \hat{P}, \hat{\phi}, \hat{p}_\phi)$ formed from our basic operators can be expanded in moments by a formal Taylor series

$$\begin{aligned} \langle\hat{O}\rangle &= \langle O(\langle\hat{V}\rangle + (\hat{V} - \langle\hat{V}\rangle), \langle\hat{P}\rangle + (\hat{P} - \langle\hat{P}\rangle), \langle\hat{\phi}\rangle + (\hat{\phi} - \langle\hat{\phi}\rangle), \langle\hat{p}_\phi\rangle + (\hat{p}_\phi - \langle\hat{p}_\phi\rangle)) \rangle \quad (9) \\ &= O(\langle\hat{V}\rangle, \langle\hat{P}\rangle, \langle\hat{\phi}\rangle, \langle\hat{p}_\phi\rangle) + \sum_{a,b,c,d} \frac{1}{a!b!c!d!} \frac{\partial^{a+b+c+d} O(\langle\hat{V}\rangle, \langle\hat{P}\rangle, \langle\hat{\phi}\rangle, \langle\hat{p}_\phi\rangle)}{\partial^a \langle\hat{V}\rangle \partial^b \langle\hat{P}\rangle \partial^c \langle\hat{\phi}\rangle \partial^d \langle\hat{p}_\phi\rangle} \Delta(V^a P^b \phi^c p_\phi^d). \end{aligned}$$

(If \hat{O} is a Weyl-ordered polynomial in basic operators, this expression is exact. If \hat{O} is not Weyl-ordered, it can be written as a sum of Weyl-ordered terms some of which have explicit factors of \hbar [28, 29]. For each of them, (9) can be used.) For the density expressions, we have

$$\langle\hat{\rho}\rangle = \frac{1}{2} \frac{\langle\hat{p}_\phi^2\rangle}{\langle\hat{V}\rangle^2} \left(1 + \frac{\Delta(p_\phi^2)}{\langle\hat{p}_\phi\rangle^2} + 3 \frac{\Delta(V^2)}{\langle\hat{V}\rangle^2} - 4 \frac{\Delta(V p_\phi)}{\langle\hat{p}_\phi\rangle \langle\hat{V}\rangle} + \dots \right) \quad (10)$$

$$\frac{\langle\hat{E}\rangle}{\langle\hat{V}\rangle} = \frac{1}{2} \frac{\langle\hat{p}_\phi^2\rangle}{\langle\hat{V}\rangle^2} \left(1 + \frac{\Delta(p_\phi^2)}{\langle\hat{p}_\phi\rangle^2} + \frac{\Delta(V^2)}{\langle\hat{V}\rangle^2} - 2 \frac{\Delta(V p_\phi)}{\langle\hat{p}_\phi\rangle \langle\hat{V}\rangle} + \dots \right) \quad (11)$$

to which fluctuations and other moments contribute in different ways.

2.2 Fluctuation energies

We extend our introductory example of the harmonic oscillator in order to discuss a general notion of fluctuation energies relevant for quantum cosmology. Equation (1) can now be

recognized as an example of the expansion (9) in terms of moments, which in this case is exact because the harmonic energy operator is a polynomial in basic operators. For a general state, the energy expectation value is obtained as the sum of the classical energy evaluated in expectation values of basic operators, and a fluctuation term. For an energy eigenstate, only the fluctuation term remains and determines the energy eigenvalue in this state.

We can derive the zero-point energy in this formalism if we consider the moments in more detail. Moments, like expectation values, are dynamical and may change in time, subject to equations of motion. Time derivatives of expectation values can be derived from the general formula

$$\frac{d\langle\hat{O}\rangle}{dt} = \frac{\langle[\hat{O}, \hat{H}]\rangle}{i\hbar} \quad (12)$$

with the Hamiltonian $\hat{H} = \hat{E}$. Moments contain products of expectation values; their time derivatives can be obtained from (12) using the Leibniz rule. For a fluctuation $\Delta(q^2) = \langle\hat{q}^2\rangle - \langle\hat{q}\rangle^2$, for instance, we have

$$\frac{d\Delta(q^2)}{dt} = \frac{\langle[\hat{q}^2, \hat{H}]\rangle}{i\hbar} - 2\langle\hat{q}\rangle \frac{\langle[\hat{q}, \hat{H}]\rangle}{i\hbar}.$$

The Hamiltonian of the harmonic oscillator implies

$$\frac{d\Delta(x^2)}{dt} = \frac{2}{m}\Delta(xp) \quad (13)$$

$$\frac{d\Delta(xp)}{dt} = \frac{1}{m}\Delta(p^2) - m\omega^2\Delta(x^2) \quad (14)$$

$$\frac{d\Delta(p^2)}{dt} = -2m\omega^2\Delta(xp). \quad (15)$$

Evaluated for a stationary state, with expectation values and moments constant in time, these equations imply that $\Delta(xp) = 0$ and $\Delta(p^2) = m^2\omega^2\Delta(x^2)$. If we also require that the uncertainty relation be saturated, as suitable for the harmonic ground state, we obtain $\Delta(x^2) = \hbar/(2m\omega)$ and the correct zero-point energy.

These considerations show that zero-point energies are just a special case of fluctuation energies as they follow from a moment expansion (9). In this form, they can be computed also for quantum cosmology, where we can use (9) to expand a constraint operator \hat{C} instead of the energy. There will then be fluctuation terms from both the gravity and the matter contribution of the constraint. The former are more sensitive to the quantization approach used, as well as to factor-ordering ambiguities.

2.3 Harmonic cosmology

The computation of fluctuation energies can be done exactly in harmonic models. Crucial ingredients, realized by the harmonic oscillator as the prime example, are a polynomial Hamiltonian for the expansion (9) to be exact, with a degree of at most two in canonical

variables. The latter property ensures that the moments obey evolution equations by which they couple only to other moments of the same order. For more-complicated systems, one can use perturbation theory provided one can find a harmonic model sufficiently close to the one of interest. (An example for a large class of such applications is the low-energy effective action for anharmonic systems [30, 27, 31].)

The harmonic oscillator is not close to all systems studied in quantum cosmology. But there are substitutes, which one may consider as harmonic models of cosmology. The procedure of canonical effective equations, based on (9) and (12), is easier to perform if one can work with a Hamiltonian rather than a constraint. We will therefore start with the technique of deparameterization, allowing one to reformulate constrained dynamics as formal evolution with respect to one of the degrees of freedom. After discussing deparameterized harmonic models, we will turn to additional ingredients required for a direct treatment of constraints.

The models of interest here can easily be deparameterized by considering the scalar ϕ as an evolution parameter. If it is free and massless, the momentum p_ϕ is a constant of motion and never becomes zero. Accordingly, the time derivative $d\phi/dt = \{\phi, C\} = p_\phi/a^3$ is non-zero, and $\phi(t)$ is a monotonic function. Instead of t , one may therefore use ϕ as a unique parameter along dynamical trajectories.

Equations of motion are then generated canonically by the function $p_\phi(Q, P)$ obtained by solving the constraint for p_ϕ : If we write the constraint as $C = \frac{1}{2}(p_\phi^2 - H(Q, P)^2)/a^3 = 0$, the Poisson-bracket relationship $dO/dt = \{O, C\}$ implies $dO/d\phi = (dt/d\phi)\{O, C\} = (a^3/p_\phi)\{O, \frac{1}{2}(p_\phi^2 - H(Q, P)^2)/a^3\} \approx \frac{1}{2}H(Q, P)^{-1}\{O, -H(Q, P)^2\} = -\{O, H(Q, P)\}$ for any expression independent of ϕ , up to terms that vanish when $C = 0$.

For the free, massless scalar in a spatially flat FRW universe, we start with the Hamiltonian constraint expressed in the canonical pair (Q, P) , which can be written as

$$\left(\frac{8\pi G(1-x)}{3}Q\right)^{-3/(2(1-x))} \left(-\frac{8\pi G}{3}(1-x)^2Q^2P^2 + \frac{1}{2}p_\phi^2\right) = 0. \quad (16)$$

It is sufficient to set the second parenthesis equal to zero (amounting to a Q -dependent choice of the time coordinate), which we do together with a simple canonical transformation from (ϕ, p_ϕ) to

$$\lambda := \sqrt{\frac{16\pi G}{3}}(1-x)\phi \quad , \quad p_\lambda = \sqrt{\frac{3}{16\pi G}} \frac{p_\phi}{1-x} \quad (17)$$

to absorb some factors. The λ -Hamiltonian p_λ is then a quadratic function $H(Q, P) = \pm|QP|$, or $\pm\delta^{-1}|Q \sin(\delta P)|$ for the loop modification. Without loss of generality, we choose the positive sign in what follows.

2.3.1 Wheeler–DeWitt model

In a Wheeler–DeWitt quantization, there are operators for both \hat{Q} and \hat{P} , and we can quantize $\hat{H} = \widehat{QP} := \frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})$ in a symmetric ordering. (For $x = 1/2$, (16) then leads to (5).) As indicated in this expression, we drop the absolute value, with the following

justification: The operator \widehat{QP} is preserved by evolution generated by $|\widehat{QP}|$. Therefore, a state initially supported on the positive part of the spectral decomposition of \widehat{QP} will always be supported on this set. For evolution equations (12) without the absolute value in \hat{H} , it is then sufficient to ensure initial states to be supported on the positive part of the spectrum, which can always be achieved by projection.

With this simplification, $\hat{H} = \hat{p}_\lambda$ is a quadratic polynomial, giving an exact expansion (9):

$$p_\lambda = \langle \hat{Q} \rangle \langle \hat{P} \rangle + \Delta(QP) \quad (18)$$

with a “fluctuation” energy $\Delta(QP)$ (which is rather a covariance). In order to see the meaning of this energy, we transform the deparameterized equation (18) back to a constraint, or an effective Friedmann equation. We compute $d\langle \hat{Q} \rangle/d\lambda = \langle \hat{Q} \rangle$ using (12). We transform the λ -derivative to a proper-time derivative by $d\langle \hat{Q} \rangle/dt = (d\langle \hat{Q} \rangle/d\lambda)(d\lambda/d\phi)(d\phi/dt)$. Finally, instead of $\langle \hat{Q} \rangle$ we introduce the effective scale factor

$$a_{\text{eff}} := \left(\frac{8\pi G}{3} (1-x) \langle \hat{Q} \rangle \right)^{1/(2(1-x))} \quad (19)$$

and write an effective Friedmann equation

$$\left(\frac{\dot{a}_{\text{eff}}}{a_{\text{eff}}} \right)^2 = \left(\frac{1}{2(1-x)} \frac{\langle \dot{\hat{Q}} \rangle}{\langle \hat{Q} \rangle} \right)^2 = \frac{4\pi G}{3} \frac{p_\phi^2}{a_{\text{eff}}^6}. \quad (20)$$

This effective Friedmann equation does not differ from the classical Friedmann equation for a free, massless scalar. The only implication of the fluctuation energy in this case is a shift from the classical p_ϕ to $p_\phi + \sqrt{16\pi G/3}(1-x)\Delta(QP)$. Since $\Delta(QP)$ is constant under evolution generated by the effective Hamiltonian (18), a constant shift of the constant of motion p_ϕ does not change the form of the dynamical equation.

For $x = -1/2$, in which case $-P = \mathcal{H}$ is the classical Hubble parameter, one could try to derive an effective Friedmann equation in a different way, by defining an effective Hubble parameter $\mathcal{H}_{\text{eff}} := -\langle \hat{P} \rangle$. Starting with (18), we could then write

$$\mathcal{H}_{\text{eff}}^2 \left(1 + \frac{\Delta(V\mathcal{H})}{a_{\text{eff}}^3 \mathcal{H}_{\text{eff}}} \right)^2 = \frac{4\pi G}{3} \frac{p_\phi^2}{a_{\text{eff}}^6} \quad (21)$$

which does have a moment term. However, even if one uses the fact that $\Delta(V\mathcal{H})$ and p_ϕ are constant, this equation is not a closed effective equation because \mathcal{H}_{eff} or $\langle \hat{P} \rangle$ is in general independent of a_{eff} or $\langle \hat{Q} \rangle$.

2.3.2 Loop model

The situation is more interesting for the constraints of loop quantum cosmology. These expressions are not polynomial in (Q, P) , but they can be made so if one transforms to non-canonical variables (Q, J) with $J := Q \exp(i\delta P)$. Our new variables can still be considered as basic ones because they form a closed algebra

$$\{Q, J\} = i\delta J \quad , \quad \{Q, J^*\} = -i\delta J^* \quad , \quad \{J, J^*\} = 2i\delta Q. \quad (22)$$

We quantize this basic algebra to

$$[\hat{Q}, \hat{J}] = -\delta\hbar\hat{J} \quad , \quad [\hat{Q}, \hat{J}^\dagger] = \delta\hbar\hat{J}^\dagger \quad , \quad [\hat{J}, \hat{J}^\dagger] = -2\delta\hbar\hat{Q}. \quad (23)$$

These commutators can be shown to follow from an ordering $\hat{J} = \widehat{\hat{Q}\exp(i\delta P)}$ up to an inconsequential shift of \hat{Q} by $\hbar/2$ [3, 32].

Instead of QP , the classical λ -Hamiltonian is then $H(Q, J) = \delta^{-1}\text{Im}J$, linear in our new variables. There is therefore no fluctuation contribution to $\langle\hat{H}\rangle = \delta^{-1}\text{Im}\langle\hat{J}\rangle$. For this operator, we can recognize the ordering in (7) by comparing it with $\hat{p}_\lambda^2 = -\frac{1}{4}\delta^{-2}(\hat{J}^2 - \hat{J}\hat{J}^\dagger - \hat{J}^\dagger\hat{J} + (\hat{J}^\dagger)^2)$ acting on eigenstates of \hat{Q} .

With a closed commutator algebra of basic operators and a linear Hamiltonian, there is no quantum back-reaction of moments coupling dynamically to expectation values. However, there is a quadratic relationship between the variables, $|J|^2 - Q^2 = 0$, in order to ensure that P contained in J is real. (It implies a Casimir constraint in the sense of [28]; see also App. A.1.2.) Upon quantization, this reality condition takes the form

$$|\langle\hat{J}\rangle|^2 - \langle\hat{Q}\rangle^2 = \Delta(Q^2) - \Delta(J\bar{J}). \quad (24)$$

If one rewrites the quantum Hamiltonian as an effective Friedmann equation, one must express $\text{Re}\langle\hat{J}\rangle$ in terms of $\langle\hat{H}\rangle$, in which process one uses (24). Fluctuation energies are thereby obtained in an indirect way. We will now show more details, but first note that moments can play crucial dynamical roles even in models that do not have quantum back-reaction. The absence of quantum back-reaction implies that equations of motion for expectation values do not couple to moments of a state, as realized in (25) below. But if there are additional constraints, such as (24), equations derived from those for basic expectation values may include moments; see (30) below.

From our Hamiltonian linear in \hat{J} we obtain an equation of motion

$$\frac{d\langle\hat{Q}\rangle}{d\lambda} = -\frac{1}{2\delta\hbar}\langle[\hat{Q}, \hat{J} - \hat{J}^\dagger]\rangle = \frac{1}{2}\langle\hat{J} + \hat{J}^\dagger\rangle = \text{Re}\langle\hat{J}\rangle. \quad (25)$$

We can use this equation to compute $d\langle\hat{Q}\rangle/dt = (d\phi/dt)(d\lambda/d\phi)(d\langle\hat{Q}\rangle/d\lambda)$ with $d\phi/dt = p_\phi/(\frac{8}{3}\pi G(1-x)\langle\hat{Q}\rangle)^{3/2(1-x)}$ as before. But first, we use the reality condition (24) in order to express $\text{Re}\langle\hat{J}\rangle$ in terms of $\text{Im}\langle\hat{J}\rangle$ and the fluctuation parameter

$$\epsilon := \frac{\Delta(Q^2) - \Delta(J\bar{J})}{\langle\hat{Q}\rangle^2}. \quad (26)$$

We obtain

$$\begin{aligned} \frac{1}{\langle\hat{Q}\rangle^2} \left(\frac{d\langle\hat{Q}\rangle}{d\phi} \right)^2 &= \frac{16\pi G}{3}(1-x)^2 \frac{(\text{Re}\langle\hat{J}\rangle)^2}{\langle\hat{Q}\rangle^2} \\ &= \frac{16\pi G}{3}(1-x)^2 \frac{\langle\hat{Q}\rangle^2 - (\text{Im}\langle\hat{J}\rangle)^2 + \epsilon\langle\hat{Q}\rangle^2}{\langle\hat{Q}\rangle^2}. \end{aligned} \quad (27)$$

We then use

$$\text{Im}\langle\hat{J}\rangle = \delta\langle\hat{H}\rangle = \sqrt{\frac{3}{16\pi G}} \frac{\delta p_\phi}{1-x}$$

and

$$\frac{(\text{Im}\langle\hat{J}\rangle)^2}{\langle\hat{Q}\rangle^2} = \frac{3}{16\pi G} \frac{\delta^2 p_\phi^2}{(1-x)^2 \langle\hat{Q}\rangle^2} = \frac{8\pi G}{3} \delta^2 \frac{p_\phi^2}{2a_{\text{eff}}^6} \left(\frac{8\pi G}{3} (1-x) \langle\hat{Q}\rangle \right)^{(1+2x)/(1-x)}.$$

Therefore,

$$\frac{1}{\langle\hat{Q}\rangle^2} \left(\frac{d\langle\hat{Q}\rangle}{d\phi} \right)^2 = \frac{16\pi G}{3} (1-x)^2 \left(1 + \epsilon - \frac{\rho_{\text{free}}}{\rho_{\text{QG}}} \right) \quad (28)$$

with

$$\rho_{\text{QG}} := \frac{3}{8\pi G \delta^2 \left(\frac{8}{3}\pi G (1-x) \langle\hat{Q}\rangle \right)^{(1+2x)/(1-x)}}. \quad (29)$$

(The energy density of the free, massless scalar is $\rho_{\text{free}} = \frac{1}{2} p_\phi^2 \left(\frac{8}{3}\pi G (1-x) \langle\hat{Q}\rangle \right)^{-3/(1-x)}$.) We finally write the equation for the proper-time derivative of a_{eff} in the form of an effective Friedmann equation

$$\begin{aligned} \left(\frac{\dot{a}_{\text{eff}}}{a_{\text{eff}}} \right)^2 &= \left(\frac{1}{2(1-x)} \frac{d\phi}{dt} \frac{d\langle\hat{Q}\rangle/d\phi}{\langle\hat{Q}\rangle} \right)^2 \\ &= \frac{8\pi G}{3} \rho_{\text{free}} \left(1 + \epsilon - \frac{\rho_{\text{free}}}{\rho_{\text{QG}}} \right) = \frac{8\pi G}{3} \left(\rho_{\text{free}} + \rho_{\text{free}} \epsilon - \frac{\rho_{\text{free}}^2}{\rho_{\text{QG}}} \right). \end{aligned} \quad (30)$$

In (30), the parameter ϵ , multiplied with ρ_{free} , plays the role of a fluctuation energy and affects the dynamics. It may seem surprising that $\rho_{\text{free}} \epsilon$ is added to the energy density, rather than just ϵ . However, using $\rho_{\text{free}} = \frac{1}{2} (d\phi/dt)^2$, we observe that there are two factors of $d\phi/dt$ in $\rho_{\text{free}} \epsilon$ which transform the fluctuation energy ϵ (or rather $\frac{1}{2}\epsilon$) from the ϕ -frame to the t -frame, according to the tensor-transformation law $\rho = T_{00} = (dt'/dt)^2 T_{0'0'} = (dt'/dt)^2 \rho'$ in isotropic models, in which only the time coordinate is being changed.

This observation highlights one of the coincidences realized for the free, massless scalar source, for which $d\phi/dt = \sqrt{2\rho_{\text{free}}}$. If there is mass term or a potential $W(\phi)$, it is not known how to generalize (30) except for perturbative derivations for small potential [23]. But it is clear that the factor of ρ_{free} multiplying the parenthesis in (30) plays different roles for the three terms: The classical Friedmann equation requires the total energy density $\rho = \rho_{\text{free}} + W(\phi)$, while ϵ should be multiplied only with ρ_{free} to provide the correct transformation of frames. For this reason, as well as the presence of quantum back-reaction, it is not easy to generalize (30) to a scalar with mass or self-interactions.

3 Applications

Our derivation of fluctuation energies in the preceding section has clarified the physical meaning of moment-dependent terms in effective equations of harmonic models. The formal

part of our calculations, however, was not new compared with previous treatments of effective equations. In this section, we use our results for two novel applications.

3.1 Instability of initial-value formulations in Euclidean regimes

The effective Friedmann equation (30) shows that $a_{\text{eff}}(t)$ has a turning point when the energy density ρ_{free} reaches the value $\rho_{\text{QG}}(1 + \epsilon)$. This turning point has been interpreted as a bounce, but since consistent inhomogeneous extensions of the background model show that space-time turns into a quantum version of 4-dimensional Euclidean space at high density, there is no deterministic evolution and the bounce picture is incorrect. Instead of using an initial-value formulation, the Euclidean phase with elliptic mode equations requires a boundary-value problem including the t -direction.

If one were to use an initial-value problem throughout the Euclidean phase, one could still find solutions to the partial differential equations for inhomogeneities. However, these solutions are not stable and depend sensitively on the initial values one selects. (Instead of oscillating Fourier terms $\exp(\pm i\omega t)$ one has exponential ones $\exp(\pm \omega t)$.) The Euclidean phase can be shown to occupy a small Planckian t -range for the harmonic model when fluctuations are small. Instabilities therefore do not make sub-Planckian fields with $\omega \ll t_{\text{P}}^{-1}$ grow much and may be assumed harmless.¹ In this section, we show that the situation changes for large fluctuations, which one should expect in a generic quantum regime likely to be realized at high density. (Our arguments indicate that a potential will have the same effect, although in this case it is more difficult to generalize the effective Friedmann equation.)

Consistent inhomogeneous extensions have been derived for the modified Friedmann equation (2), which follows from a modified constraint

$$C_{\text{mod}} = -\frac{3}{8\pi G}V\frac{\sin^2(\delta P)}{\delta^2} + \frac{p_\phi^2}{2V} = 0 \quad (31)$$

assuming $x = -1/2$ and referring to the pair (V, P) with $\{V, P\} = 4\pi G$. Indeed, if we compute $\dot{V} = \{V, C_{\text{mod}}\} = -3V \sin(2\delta P)/2\delta$, we have $\mathcal{H}^2 = (\frac{1}{3}\dot{V}/V)^2 = \delta^{-2}(\sin^2(\delta P) - \sin^4(\delta P)) = (8\pi G/3)\rho_{\text{free}}(1 - \rho_{\text{free}}/\rho_{\text{QG}})$. Alternatively, we can write this equation as $\sin^2(\delta P) = \rho_{\text{free}}/\rho_{\text{QG}}$. For a background dynamics subject to this modification, consistent mode equations have the speed $\beta = \cos(2\delta P) = 1 - 2\rho_{\text{free}}/\rho_{\text{QG}}$ [6, 33]. More generally, if the term \mathcal{H}^2 in the classical Friedmann equation is replaced by some function $f(V, P)$ with \mathcal{H}^2 as the limit for $\delta \rightarrow 0$, the speed of modes in consistent inhomogeneous models is given by

$$\beta = \frac{1}{2}\partial^2 f / \partial P^2. \quad (32)$$

This general form, derived for spherically symmetric models [5, 7], is consistent with the results of [6, 33]. When $\beta < 0$, mode equations become elliptic and the space-time signature

¹This possibility has been pointed out by Jaume Garriga.

turns Euclidean. In cosmological models based on (2), the density at the transition point is half the maximum density, $\frac{1}{2}\rho_{\text{QG}}$.

Consistent versions of inhomogeneous equations have not yet been derived in the presence of moment terms and quantum back-reaction, and we cannot easily extend these conclusions about signature change to the effective Friedmann equation (30) when the fluctuation energy ϵ is large. Fortunately, however, the general form of the relationship (32) allows us to estimate the behavior with just a few reasonable assumptions.

For a consistent set of equations, the moment dependence of background and mode equations is likely to be restricted. Without knowing the precise dependence, we only assume that the modification function in the constraint

$$C_{\text{mod}} = -\frac{3}{8\pi G}Vf(V, P, \Delta(\cdot)) + V\rho_{\text{free}} = 0 \quad (33)$$

is now allowed to depend also on moments $\Delta(\cdot)$ of the pair (V, P) . If the dependence of f on V is not very strong, we still have a monotonic function $P(t)$ because

$$\frac{dP}{dt} = \{P, C_{\text{mod}}\} = \frac{3}{2} \left(f + V \frac{\partial f}{\partial V} \right) + 2\pi G \frac{p_\phi^2}{V^2} \approx 2f + \frac{3}{2}V \frac{\partial f}{\partial V} > 0 \quad (34)$$

as long as $\partial f/\partial V$ is sufficiently small. (We have $f = (8\pi G/3)\rho_{\text{free}} > 0$ when $C_{\text{mod}} = 0$.) With (32), β is therefore negative when $\partial f/\partial P$ decreases in time.

The change of $\partial f/\partial P$ in time is related to the behavior of the effective Hubble parameter: we have $\dot{a}_{\text{eff}}/a_{\text{eff}} = \frac{1}{3}\dot{V}/V = \{V, C_{\text{mod}}\}/3V = -\frac{1}{2}\partial f/\partial P$. We can then write

$$\beta = \frac{1}{2}\partial^2 f/\partial^2 P = -d(\dot{a}_{\text{eff}}/a_{\text{eff}})/dP. \quad (35)$$

All we need to do to determine the density range of the Euclidean phase is to discuss the behavior of the effective Hubble parameter in relation to the energy density, as given by the effective Friedmann equation.

In a collapse phase, the energy density increases and approaches $\rho_{\text{QG}}(1 + \epsilon)$. For sufficiently small densities, $-\dot{a}_{\text{eff}}/a_{\text{eff}}$ is positive and increases until $\delta^2(\dot{a}_{\text{eff}}/a_{\text{eff}})^2 = (\rho_{\text{free}}/\rho_{\text{QG}})(1 + \epsilon - \rho_{\text{free}}/\rho_{\text{QG}})$ reaches a maximum as a function of $\rho_{\text{free}}/\rho_{\text{QG}}$. From then on, $-\dot{a}_{\text{eff}}/a_{\text{eff}}$ decreases with P and β becomes negative according to (35). The maximum is reached when $\rho_{\text{free}} = \frac{1}{2}\rho_{\text{QG}}(1 + \epsilon)$, that is at half the maximum density where $\dot{a}_{\text{eff}}/a_{\text{eff}} = 0$. When the density is between $\frac{1}{2}\rho_{\text{QG}}(1 + \epsilon)$ and $\rho_{\text{QG}}(1 + \epsilon)$, the signature is of Euclidean type.

The harmonic model provides solutions $\langle \hat{V} \rangle(\phi) \propto \cosh(\phi)$ [3]. (See also App. A.3.1.) For the free density $\frac{1}{2}p_\phi^2/\langle \hat{V} \rangle^2$ to change from $\frac{1}{2}\rho_{\text{QG}}(1 + \epsilon)$ to $\rho_{\text{QG}}(1 + \epsilon)$ (with constant p_ϕ), we need $\cosh(\phi)$ to change by a factor of the order one. Therefore, t changes by an amount Δt which is a number of order one times the (nearly constant) value of $dt/d\phi = 1/\sqrt{2\rho_{\text{free}}}$ in this small ϕ -interval. In the given density range, we have $\rho_{\text{free}} \sim \rho_{\text{QG}}(1 + \epsilon)$. If fluctuations are significant and $\epsilon < 0$, ρ_{free} can be well below the Planck density even if $\rho_{\text{QG}} \sim \rho_{\text{P}}$. (In the next section we will show that ϵ is negative for a Gaussian in V .) Accordingly, the t -range of the Euclidean phase is much larger than the ϕ -range, which is of order one.

Quantum fluctuations can enlarge the size of the Euclidean phase, so that instabilities of an initial-value formulation are relevant not only for trans-Planckian modes. Only a boundary-value formulation for elliptic equations can avoid these instabilities.

3.2 Comparisons with numerical results

If one solves differential or difference equations numerically, one must assume an initial wave function. Unfortunately, quantum cosmology does not give rise to a strongly restricted class of states. Gaussians in some variables are usually justified in near-vacuum considerations of perturbative field theories, just because the free vacuum happens to be Gaussian. Quantum cosmology, with its unbounded-from-below gravitational contribution to the Hamiltonian constraint, does not imply a clear ground state, let alone a near-Gaussian one. And although Gaussians provide nice semiclassical states, a general semiclassical regime may require a larger class of states (perhaps even mixed ones). In models with relevant quantum back-reaction or fluctuation energies, the form of the state matters because it determines the moments.

Nevertheless, provided one interprets them carefully enough in the light of quantization ambiguities and state choices, numerical solutions can provide valuable insights. In this section, we discuss several examples of fluctuation effects which can be derived easily from effective equations and be compared with existing numerical results.

3.2.1 Fluctuation energy

Our expression for the fluctuation energy in (30), given by (26), is valid for any state. We illustrate its effects more explicitly by computing the value for two classes of states, both Gaussian but with respect to different canonical variables.

Gaussian in the volume. Given the expression of ϵ in terms of (V, P) -moments, one can rather easily compute it for a Gaussian state in Q , with wave function

$$\psi(Q) = \frac{1}{(2\pi)^{1/4} \sqrt{\sigma}} \exp\left(-\frac{(Q - \bar{Q})^2}{4\sigma^2}\right) \exp(i\hbar^{-1} \bar{P}Q). \quad (36)$$

(For all wave functions, we refer to standard L^2 -Hilbert spaces. Since we have deparameterized by ϕ or λ , these are physical Hilbert spaces.) The Q -fluctuation $\Delta Q = \sigma$ and the expectation values \bar{Q} and \bar{P} of \hat{Q} and \hat{P} are well-known.

Using $\hat{J} = \hat{Q} \exp(i\delta P)$, with the exponential acting as a shift operator on $\psi(Q)$, we compute

$$\langle \hat{J} \rangle = (\bar{Q} - \tfrac{1}{2}\delta\hbar) \exp(-\tfrac{1}{8}\sigma^{-2}\delta^2\hbar^2 + i\bar{P}\delta) \quad (37)$$

and

$$\Delta(J\bar{J}) = \sigma^2 + \bar{Q}(\bar{Q} - \delta\hbar) (1 - \exp(-\delta^2\hbar^2/4\sigma^2)) + \tfrac{1}{2}\delta^2\hbar^2 \left(1 - \tfrac{1}{2} \exp(-\delta^2\hbar^2/4\sigma^2)\right). \quad (38)$$

For $2\sigma \gg \delta\hbar$ (a Q -fluctuation much larger than the discrete spacing of Q), we can expand the exponentials and obtain

$$\epsilon = -\frac{1}{4} \frac{\delta^2 \hbar^2}{\sigma^2} = -\frac{1}{4} \frac{\delta^2 \hbar^2}{(\Delta Q)^2} = -\frac{4\pi^2 \delta^2 \ell_P^4}{(\Delta V)^2}, \quad (39)$$

the last part for $x = -1/2$.

The fluctuation energy for a Q -Gaussian is inversely proportional to the squared Q -fluctuation and grows for small ΔQ , and it is negative. For a comparison with [13] (using $x = -1/2$), it is useful to replace the dependence on ΔV only by a dependence on the two parameters $\Delta V/\langle \hat{V} \rangle$ and p_ϕ , writing

$$\epsilon = -\frac{3\pi G \hbar^2}{p_\phi^2} \left(\frac{\langle \hat{V} \rangle}{\Delta V} \right)^2 \frac{\rho_{\text{free}}}{\rho_{\text{QG}}}. \quad (40)$$

If $\Delta V/\langle \hat{V} \rangle$ and p_ϕ are treated as independent variables, ϵ depends on ρ_{free} . Our previous equation for the maximum effective density, $\rho_{\text{free}}^{\text{max}} = \rho_{\text{QG}}(1 + \epsilon)$, can then be solved for

$$\rho_{\text{free}}^{\text{max}} = \frac{\rho_{\text{QG}}}{1 + \frac{3\pi G \hbar^2}{p_\phi^2} \left(\frac{\langle \hat{V} \rangle}{\Delta V} \right)^2}. \quad (41)$$

See Fig. 1.

Slightly more generally, we can allow for correlations of the pair (Q, P) , amounting to a fully squeezed state with wave function

$$\psi(Q) = \frac{1}{(2\pi)^{1/4} \sqrt{\sigma}} \exp \left(-\frac{(Q - \bar{Q})^2}{4\sigma^2} (1 - 2i\kappa/\hbar) \right) \exp(i\hbar^{-1} \bar{P}Q) \quad (42)$$

with the covariance $\kappa = \Delta(QP)$. We still have $\Delta Q = \sigma$, but κ contributes to the momentum fluctuation $\Delta P = \frac{1}{2}\hbar\sqrt{1 + 4\kappa^2/\hbar^2}/\sigma$.

Proceeding as before, we now have

$$\begin{aligned} \Delta(J\bar{J}) &= \sigma^2 + \bar{Q}(\bar{Q} - \delta\hbar) (1 - \exp(-\delta^2 \hbar^2 (1 + 4\kappa^2/\hbar^2)/4\sigma^2)) \\ &\quad + \frac{1}{2} \delta^2 \hbar^2 \left(1 - \frac{1}{2} (1 + 4\kappa^2/\hbar^2) \exp(-\delta^2 \hbar^2 (1 + 4\kappa^2/\hbar^2)/4\sigma^2) \right). \end{aligned}$$

The dominant contribution to ϵ receives an additional factor of $1 + 4\kappa^2/\hbar^2$. As this factor is always positive, correlations do not change the fact that a Gaussian in the volume does not increase the maximum density beyond ρ_{QG} . The graph of $\rho_{\text{free}}^{\text{max}}$ is as in Fig. 1 but with values $p_\phi/\sqrt{1 + 4\kappa^2/\hbar^2}$ instead of p_ϕ .

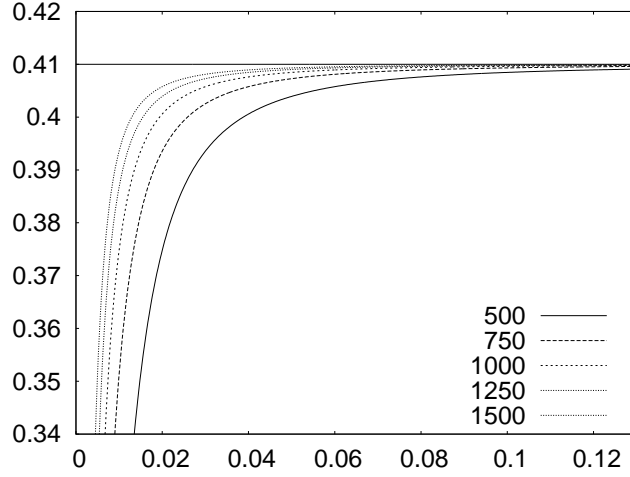


Figure 1: The maximal effective density (41) as a function of $\Delta V/\langle\hat{V}\rangle$, for different values of p_ϕ . The parameter $\rho_{\text{QG}} \approx 0.41$ (in units with $G = 1 = \hbar$) has been chosen to be close to the one used in [13]. (This choice amounts to $\delta = 2\sqrt{\pi}\sqrt[4]{3}\gamma^{3/2}$ with the Barbero–Immirzi parameter $\gamma = 0.238$ [34, 35], as it follows from a comparison of the general (and non-unique) step-size 2δ in (7) with the specific choice made in [13].) This plot is to be compared with Fig. 15 of [13].

Gaussian in the scalar. In [2] and [13], an alternative wave function has been used as an initial state in a regime in which the Wheeler–DeWitt equation is valid, which amounts to a Gaussian as well but in (ϕ, p_ϕ) rather than (Q, P) . It has the form

$$\psi(Q) = \sqrt{\frac{\sigma/2}{\sqrt{2\pi}|Q|}} \exp\left(-\frac{1}{4}\sigma^2(\log|Q/\bar{Q}|)^2\right) \exp(i\bar{p}_\lambda \log(|Q/\bar{Q}|)/\hbar) \quad (43)$$

in a slightly modified notation. If (43) is used as a state in the loop-quantized model, the inner product is initially defined by summation over a discrete subset of all Q , but for states spread more widely than $\delta\hbar$ the summation is well approximated by an integral.

In a quantum model deparameterized by ϕ or λ it is, in general, not meaningful to speak of a Gaussian in (λ, p_λ) . Moreover, there are no operators for $\hat{\lambda}$ and \hat{p}_λ , and correspondingly no expectation values and moments for these variables. However, in an initial-state regime in which the Wheeler–DeWitt equation is valid and the evolved state remains semiclassical, a λ -Gaussian $\psi(Q)$ may be defined in $\lambda(Q) = \log|Q/\bar{Q}| + \bar{\lambda}$, the classical solution for λ . This definition leads to (43). As for operators, one can use the constraint equation to replace $\hat{p}_\lambda\psi = -i\hbar\partial\psi/\partial\lambda$ by $\widehat{QP}\psi$, and $\hat{\lambda}$ as a multiplication operator with the classical solution $\lambda(Q) = \log|Q/\bar{Q}| + \bar{\lambda}$. With these prescriptions, we obtain

$$\langle\hat{\lambda}\rangle = \bar{\lambda} \quad , \quad \langle\hat{p}_\lambda\rangle = \bar{p}_\lambda \quad , \quad \Delta\lambda = \frac{1}{\sigma} \quad , \quad \Delta p_\lambda = \frac{1}{2}\hbar\sigma \quad (44)$$

for a wave function (43).

Moreover, in the standard way of a Q -representation of wave functions we compute the expectation value

$$\langle \hat{Q} \rangle = \frac{\sigma}{\sqrt{2\pi}} \int_0^\infty \exp\left(-\frac{\sigma^2}{2}(\log(Q/\bar{Q}))^2\right) dQ = \bar{Q} \exp(1/2\sigma^2). \quad (45)$$

(The integration can easily be performed after substituting $\lambda = \log(Q/\bar{Q})$, so that also here we are formally writing the wave function as a Gaussian in the scalar.) A similar calculation gives

$$\Delta(Q^2) = \bar{Q}^2 \left(e^{2/\sigma^2} - e^{1/\sigma^2} \right) = \langle \hat{Q} \rangle^2 (e^{1/\sigma^2} - 1). \quad (46)$$

In order to compute expectation values containing shift operators, such as $\langle \hat{J} \rangle$, we may expand in $\delta\hbar/Q$ before integrating, which is reasonable in the same regime in which the inner product can be written as an integral. However, we must be careful because the momentum term $\exp(i\hbar^{-1}\bar{p}_\lambda \log |(Q + \delta\hbar)/\bar{Q}|)$, after the logarithm is expanded in $\delta\hbar/Q$, gives rise to terms of the order $\delta\bar{p}_\lambda/Q$ which are not small near the bounce regime. Nevertheless, it may be of interest to expand in $\delta\bar{p}_\lambda/Q$ for analytic integrations in the form of polynomials times Gaussians. When applied to an initial state, the volume spread should therefore be sufficiently small to keep the support of the wave function away from $Q \sim \delta\bar{p}_\lambda$.

In this way, we find

$$\langle \hat{J} \rangle = \langle \hat{Q} \rangle - \frac{1}{2}\delta\hbar + i\delta\bar{p}_\lambda \quad (47)$$

(note that $\text{Im}\langle \hat{J} \rangle = \delta\bar{p}_\lambda$, consistent with $\langle \hat{p}_\lambda \rangle = \bar{p}_\lambda$) and the final moment

$$\Delta(J\bar{J}) = \langle \hat{Q}^2 \rangle - \delta\hbar\langle \hat{Q} \rangle - |\langle \hat{J} \rangle|^2. \quad (48)$$

The fluctuation energy in this case is

$$\epsilon = \frac{\delta^2\bar{p}_\lambda^2}{\langle \hat{Q} \rangle^2} = \frac{4\pi G}{3} \frac{\delta^2 p_\phi^2}{\langle \hat{V} \rangle^2} = \frac{\rho_{\text{free}}}{\rho_{\text{QG}}}, \quad (49)$$

the latter relations for $x = -1/2$. Surprisingly, the fluctuation energy (which is now positive) cancels the term produced by holonomy modifications in the Friedmann equation. (The next-order contribution $4\pi^2\delta^2\ell_{\text{P}}^2/\langle \hat{V} \rangle^2$ is very small.) Moment terms are thereby shown to be able to rival holonomy modifications of loop quantum cosmology. If such a state were realized for an extended period of evolution at high density (as opposed to initially as assumed in [2, 13]), the volume expectation value could avoid a bounce. But again, our approximation of the integrations in $\Delta(J\bar{J})$, especially in $\text{Re}\langle \hat{J} \rangle$, is not expected to be good at high density.

Also here, we can repeat our calculations for fully squeezed states with wave function

$$\psi(Q) = \sqrt{\frac{\sigma/2}{\sqrt{2\pi}|Q|}} \exp\left(-\frac{1}{4}\sigma^2(\log |Q/\bar{Q}|)^2(1 - 2i\kappa/\hbar)\right) \exp(i\bar{p}_\lambda \log(|Q/\bar{Q}|)/\hbar). \quad (50)$$

In this case, we find that the fluctuation energy does not depend on κ .

3.2.2 Effective constraints and relations between moments

So far, we have mainly considered deparameterized equations. After deparameterization, the “time” part of the system, given here by (ϕ, p_ϕ) or (λ, p_λ) , is not fully quantized, and information about moments containing one or more of these variables is partially lost. We have to go back to the original constrained system in order to retrieve this information, while making sure that the constraints are satisfied for physical states. The formalism of effective constraints, developed in [36, 37], is useful for this task.

A constraint operator \hat{C} , such as

$$\hat{C} = \delta^2 \hat{p}_\lambda^2 - (Q \widehat{\sin(\delta P)})^2 \quad (51)$$

as used for (7), gives rise to an effective constraint $\langle \hat{C} \rangle$ which can be expanded in expectation values and moments just like an effective Hamiltonian, using (9). However, solving $\langle \hat{C} \rangle = 0$ is not sufficient because a vanishing expectation value of \hat{C} in some state does not imply that the state is annihilated by \hat{C} . As shown in [36, 37], a complete and consistent (first-class) constrained system is obtained if one accompanies $\langle \hat{C} \rangle$ by infinitely many effective constraints $C_{\text{pol}} := \langle \widehat{\text{pol}} \hat{C} \rangle$ for polynomials $\widehat{\text{pol}}$ in $\hat{O} - \langle \hat{O} \rangle$ for all basic operators \hat{O} . To finite order in the moments, a finite number of effective constraints is sufficient.

As basic operators appropriate for (51), we choose $(\hat{Q}, \widehat{\sin(\delta P)}, \widehat{\cos(\delta P)})$. There will then be moments involving powers of all three operators. However, they are not all independent if we impose the constraint

$$\hat{T}\psi := \left(\widehat{\sin(\delta P)}^2 + \widehat{\cos(\delta P)}^2 - 1 \right) \psi = 0 \quad (52)$$

so that $\langle \widehat{\exp(i\delta P)} \rangle = \langle \widehat{\cos(\delta P)} \rangle + i \langle \widehat{\sin(\delta P)} \rangle$ is unitary. We then have two constraint operators, \hat{C} and \hat{T} , but since \hat{T} is a Casimir operator and commutes with all constraints it is easier to solve [28]. (The Casimir property also implies that \hat{C} and \hat{T} form a pair of first-class constraints.) There is no gauge flow associated with effective constraints of \hat{T} , but only relations between moments. For instance, for second-order moments we have a general relationship $\langle \widehat{\sin(\delta P)} \rangle \Delta(\sin(\delta P) \cdots) + \langle \widehat{\cos(\delta P)} \rangle \Delta(\cos(\delta P) \cdots) = 0$ which allows us to eliminate all moments involving $\cos(\delta P)$. See App. A.1.2 for more details.

We will be interested in second-order moments, for which we include

$$\begin{aligned} \langle \hat{C} \rangle &= \delta^2 \langle \hat{p}_\lambda^2 \rangle - \langle \hat{Q} \rangle^2 \langle \widehat{\sin(\delta P)} \rangle^2 + \delta^2 \Delta(p_\lambda^2) - \langle \widehat{\sin(\delta P)} \rangle^2 \Delta(Q^2) - \langle \hat{Q} \rangle^2 \Delta(\sin(\delta P)^2) \\ &\quad - 4 \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \Delta(Q \sin(\delta P)) \end{aligned} \quad (53)$$

and constraints C_{pol} with linear polynomials. (We ignore re-ordering terms which would have explicit factors of \hbar .) We will not need C_λ here, but do use

$$\begin{aligned} C_{p_\lambda} &= 2\delta^2 \langle \hat{p}_\lambda \rangle \Delta(p_\lambda^2) - 2 \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \Delta(p_\lambda Q) - 2 \langle \hat{Q} \rangle^2 \langle \widehat{\sin(\delta P)} \rangle \Delta(p_\lambda \sin(\delta P)) \\ C_Q &= 2\delta^2 \langle \hat{p}_\lambda \rangle \Delta(p_\lambda Q) - 2 \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle^2 \Delta(Q^2) \end{aligned} \quad (54)$$

$$-2\langle\hat{Q}\rangle^2\langle\widehat{\sin(\delta P)}\rangle\left(\Delta(Q\sin(\delta P)) + \frac{1}{2}i\hbar\delta\langle\widehat{\cos(\delta P)}\rangle\right) \quad (55)$$

$$\begin{aligned} C_{\sin(\delta P)} &= 2\delta^2\langle\hat{p}_\lambda\rangle\Delta(p_\lambda\sin(\delta P)) - 2\langle\hat{Q}\rangle\langle\sin(\delta\hat{P})\rangle^2\left(\Delta(Q\sin(\delta P)) - \frac{1}{2}i\hbar\delta\langle\widehat{\cos(\delta P)}\rangle\right) \\ &\quad - 2\langle\hat{Q}\rangle^2\langle\widehat{\sin(\delta P)}\rangle\Delta(\sin(\delta P)^2). \end{aligned} \quad (56)$$

If we solve $C_Q = 0$ and $C_{\sin(\delta P)} = 0$ for $\Delta(p_\lambda Q)$ and $\Delta(p_\lambda \sin(\delta P))$ and insert the results in the solution for $\Delta(p_\lambda^2)$ obtained from $C_{p_\lambda} = 0$, we find

$$\Delta(p_\lambda^2) = \langle\hat{p}_\lambda\rangle^2\frac{\Delta(Q^2)}{\langle\hat{Q}\rangle^2} + \frac{2\langle\hat{p}_\lambda\rangle}{\delta}\Delta(Q\sin(\delta P)) + \frac{\langle\hat{Q}\rangle^2}{\delta^2}\Delta(\sin(\delta P)^2) \quad (57)$$

using that (53) implies $\langle\hat{Q}\rangle^2\langle\widehat{\sin(\delta P)}\rangle^2 = \delta^2\langle\hat{p}_\lambda\rangle^2 + O(\Delta(\cdot))$ and suppressing quadratic terms in second-order moments along with higher-order ones. (Owing to imaginary contributions in the effective constraints C_Q and $C_{\sin(\delta P)}$, the moments $\Delta(p_\lambda Q)$ and $\Delta(p_\lambda \sin(\delta P))$ are complex. We discuss this feature in the appendix.)

Gaussian in the volume. For an uncorrelated Gaussian

$$\psi(Q) = \frac{1}{\sqrt[4]{2\pi}\sqrt{\sigma}} \exp\left(-\frac{(Q - \bar{Q})^2}{4\sigma^2}\right) \exp(i\bar{P}Q/\hbar), \quad (58)$$

we have $\Delta(Q\sin(\delta P)) = 0$ and

$$\delta^{-2}\Delta(\sin(\delta P)^2) = \langle\widehat{\cos(\delta P)}\rangle^2\Delta(P^2) = \left(1 - \frac{\delta^2\langle\hat{p}_\lambda\rangle^2}{\langle\hat{Q}\rangle^2} + O(\Delta(\cdot))\right) \frac{\hbar^2}{4\Delta(Q^2)}. \quad (59)$$

In this case, using (57),

$$\Delta p_\lambda = \sqrt{\frac{\hbar^2}{4}\frac{\langle\hat{Q}\rangle^2}{\Delta(Q^2)} + \langle\hat{p}_\lambda\rangle^2\left(\frac{\Delta(Q^2)}{\langle\hat{Q}\rangle^2} - \frac{\delta^2\hbar^2}{4\Delta(Q^2)}\right)} \quad (60)$$

or (for $x = -1/2$)

$$\Delta p_\phi = \sqrt{3\pi G\hbar^2\frac{\langle\hat{V}\rangle^2}{(\Delta V)^2} + \langle\hat{p}_\phi\rangle^2\left(\frac{(\Delta V)^2}{\langle\hat{V}\rangle^2} - \frac{4\pi^2\delta^2\ell_P^4}{(\Delta V)^2}\right)}. \quad (61)$$

The last contribution can be written as $-3\pi G\hbar^2(\rho_{\text{eff}}/\rho_{\text{QG}})\langle\hat{V}\rangle^2/(\Delta V)^2$ and is therefore small compared to the first term for an initial state. Ignoring the last contribution, Δp_ϕ is plotted as a function of $\Delta V/\langle\hat{V}\rangle$ in Fig. 2. For small $\Delta V/\langle\hat{V}\rangle$, the first term is dominant and Δp_ϕ is independent of $\langle\hat{p}_\phi\rangle$. We can also see that

$$\frac{\Delta V}{\langle\hat{V}\rangle}\Delta p_\phi = \sqrt{3\pi G\hbar^2 + \langle\hat{p}_\phi\rangle^2\left(\frac{\Delta V}{\langle\hat{V}\rangle}\right)^4 - 4\pi^2\delta^2\ell_P^4\frac{\langle\hat{p}_\phi\rangle^2}{\langle\hat{V}\rangle^2}} \quad (62)$$

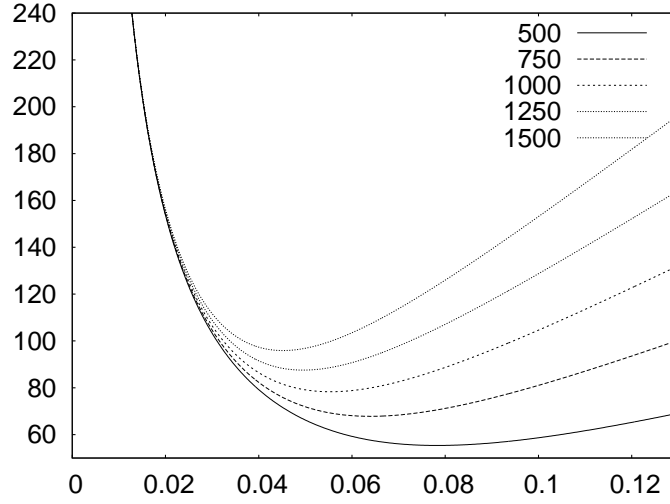


Figure 2: The p_ϕ -fluctuation (61) as a function of $\Delta V/\langle\hat{V}\rangle$, for different values of p_ϕ . Other parameters are as in Fig. 1. This plot is to be compared with Fig. 11 of [13].

is bounded from below by $\sqrt{3\pi G\hbar}$, noting that the last term is small when the volume expectation value is larger than Planckian. The minimum value $(\Delta p_\phi)_{\min}^2 = 2\sqrt{3\pi G\hbar}p_\phi$ is obtained for $(\Delta V/\langle\hat{V}\rangle)^2 = \sqrt{3\pi G\hbar}/p_\phi$. Some of these limiting cases have been mentioned in [13].

For a correlated Gaussian, we obtain

$$\Delta p_\phi = \sqrt{3\pi G\hbar^2(1 + 4\kappa^2/\hbar^2)\frac{\langle\hat{V}\rangle^2}{\Delta(V^2)}\left(1 - \frac{\rho_{\text{free}}}{\rho_{\text{QG}}}\right) + \langle\hat{p}_\phi\rangle^2\left(\frac{\Delta(V^2)}{\langle\hat{V}\rangle^2} + 2\frac{\Delta(VP)}{\langle\hat{V}\rangle\langle\hat{P}\rangle}\right)}. \quad (63)$$

At small curvature (appropriate for an initial state at large volume), we can write the last contribution as $2\langle\hat{p}_\phi\rangle^2\Delta(VP)/\langle\hat{V}\rangle\langle\hat{P}\rangle = 4\sqrt{3\pi G\hbar^2}\langle\hat{p}_\phi\rangle\kappa/\hbar$. In this form, the behavior of Δp_ϕ is shown in Fig. 3. Effects of $\kappa \neq 0$ are largest around the minimum of $\Delta V/\langle\hat{V}\rangle$ as a function of Δp_ϕ .

Gaussian in the scalar. A state in the volume representation which is Gaussian for the field value is of the form (43). In addition to expectation values and moments computed before, we have

$$\langle\widehat{\sin(\delta P)}\rangle = \frac{\delta\bar{p}_\lambda}{Q}e^{1/2\sigma^2} \quad (64)$$

and

$$\Delta(Q^2) = \bar{Q}^2(e^{2/\sigma^2} - e^{1/\sigma^2}) = \langle\hat{Q}\rangle^2(e^{1/\sigma^2} - 1) \quad (65)$$

$$\Delta(Q\sin(\delta P)) = \delta\bar{p}_\lambda(1 - e^{1/\sigma^2}) \quad (66)$$

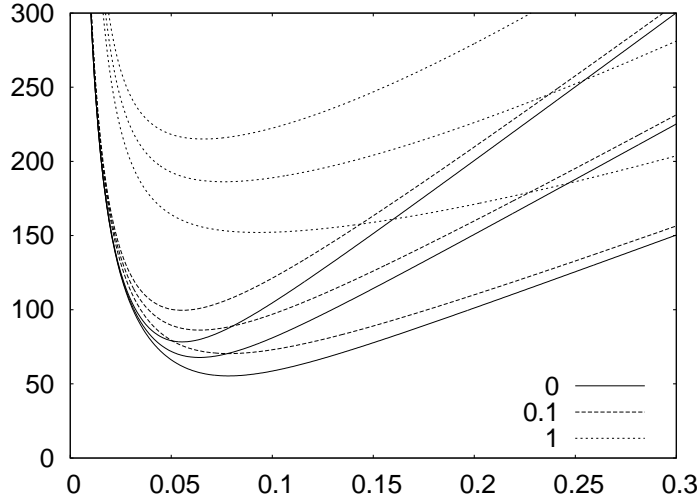


Figure 3: The p_ϕ -fluctuation (63) as a function of $\Delta V/\langle\hat{V}\rangle$, for different values of p_ϕ and κ (as shown in units of \hbar). Other parameters are as in Fig. 1.

$$\Delta(\sin(\delta P)^2) = 3\frac{\delta^2\hbar^2}{Q^2}\left(\frac{\sigma^2}{4} + 1\right)e^{2/\sigma^2} + \frac{\delta^2\bar{p}_\lambda^2}{Q^2}\left(4(1 + 4/\sigma^4)e^{2/\sigma^2} - 1\right). \quad (67)$$

Our moment relations derived from effective constraints then imply

$$\Delta p_\phi = \sqrt{36\pi G\hbar^2\left(\frac{\sigma^2}{4} + 1\right)e^{3/\sigma^2} + \langle\hat{p}_\phi\rangle^2\left(4\left(1 + \frac{4}{\sigma^2}\right)e^{3/\sigma^2} - 2e^{1/\sigma^2} + 1\right)}. \quad (68)$$

For small $\Delta V/\langle\hat{V}\rangle$ (large σ), the most relevant term is $\Delta(p_\phi)^2 \sim 9\pi G\hbar^2\sigma^2 \sim 9\pi G\hbar^2(\langle\hat{V}\rangle/\Delta V)^2$, which is independent of $\langle\hat{p}_\phi\rangle$. Moreover, Δp_ϕ is inversely proportional to $\Delta V/\langle\hat{V}\rangle$.

As noted before, we must be careful with the expansions used here for integrations when volume fluctuations are not sufficiently small. Fortunately, the relation between ΔV and Δp_ϕ can be obtained more easily from a combination of Eqs. (44) and (46): With $\sigma = 2\Delta p_\lambda/\hbar = (3\pi G\hbar^2)^{-1/2}\Delta p_\phi$, we obtain

$$\frac{\Delta V}{\langle\hat{V}\rangle} = \sqrt{\exp\left(\frac{3\pi G\hbar^2}{(\Delta p_\phi)^2}\right) - 1} \quad (69)$$

which equals $\exp(\frac{3}{2}\pi G\hbar^2/(\Delta p_\phi)^2)$ for $\Delta p_\phi \ll 3\pi G\hbar^2$, and $\sqrt{3\pi G\hbar^2}/\Delta p_\phi$ for $\Delta p_\phi \gg 3\pi G\hbar^2$. The full function is shown in Fig. 4. Notice that $\Delta p_\phi\Delta V/\langle\hat{V}\rangle$ is a constant (equal to $\sqrt{3\pi G\hbar^2}$) for small relative volume fluctuations, so that setting $\Delta Q/\langle\hat{Q}\rangle \approx \Delta\lambda$ is consistent with the saturation of the (λ, p_λ) -uncertainty relation for the Gaussian (43), as remarked in [13]. For large values, $\Delta Q/\langle\hat{Q}\rangle$ is no longer proportional to $\Delta\lambda$ as the classical solutions, identifying λ with $\log(Q/\bar{Q}) + \bar{\lambda}$, would suggest. The minimal-uncertainty Gaussian in the

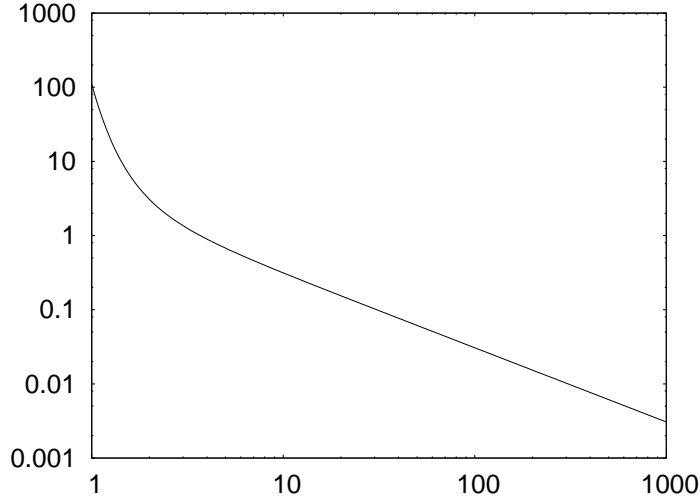


Figure 4: The relative volume fluctuation (69) as a function of Δp_ϕ , for arbitrary values of p_ϕ . Other parameters are as in Fig. 1. This plot is to be compared with Fig. 16 of [13].

scalar therefore may lead to larger values of $\Delta V/\langle\hat{V}\rangle$ than expected from an identification of this relative fluctuation with $\Delta\lambda$.

For a squeezed state, we have the previous expression (46) for ΔQ in terms of σ , but now $\Delta p_\lambda = \frac{1}{2}\hbar\sigma\sqrt{1+4\kappa^2/\hbar^2}$. Thus,

$$\frac{\Delta V}{\langle\hat{V}\rangle} = \sqrt{\exp\left(\frac{3\pi G\hbar^2}{(\Delta p_\phi)^2}(1+4\kappa^2/\hbar^2)\right) - 1}. \quad (70)$$

Different values of $\kappa \neq 0$ simply shift the curve in Fig. 4 up.

3.2.3 Density operator

The fluctuation energy is relevant for the maximum density reached along solutions to the Hamiltonian constraint of the harmonic model. According to (39), departures from ρ_{QG} are largest for small volume fluctuations. However, a second source of volume fluctuations matters for a comparison of evolved densities with the value ρ_{QG} : Depending on what expression is used to compute density expectation values, additional moments may appear as in (10).

As shown in [25], the density operator $\hat{\rho} = \frac{1}{2}\hat{p}_\phi^2\hat{V}^{-2}$ has a continuous spectrum bounded by ρ_{QG} in models of loop quantum cosmology, irrespective of the precise factor ordering of the constraint. Although the expectation value $\langle\hat{\rho}\rangle$ in a specific evolved state may not necessarily reach this bound (or may even be larger if there are discrete eigenvalues of $\hat{\rho}$ above ρ_{QG}), the value of ρ_{QG} sets a distinguished scale in this problem.

Effective equations, such as (30), contain density parameters. However, as seen from the detailed derivation in Section 2.3.2, these effective densities are defined as $\rho_{\text{eff}} =$

$\frac{1}{2}\langle\hat{p}_\phi\rangle^2/\langle\hat{V}\rangle^2$, not as $\langle\hat{\rho}\rangle$. We can then write (10) as an expression that relates the effective density to the density expectation value:

$$\rho_{\text{eff}} = \frac{\langle\hat{\rho}\rangle}{1 + \frac{\Delta(p_\phi^2)}{\langle\hat{p}_\phi\rangle^2} + 3\frac{\Delta(V^2)}{\langle\hat{V}\rangle^2} - 4\frac{\Delta(Vp_\phi)}{\langle\hat{p}_\phi\rangle\langle\hat{V}\rangle} + \dots}. \quad (71)$$

We ignore higher-order moments for semiclassical states, but they may contribute for larger volume fluctuations.

The remaining moments are all related to the volume fluctuation, as shown in the preceding subsection: For an uncorrelated V -Gaussian,

$$\frac{(\Delta p_\phi)^2}{\langle\hat{p}_\phi\rangle^2} = \frac{(\Delta V)^2}{\langle\hat{V}\rangle^2} + \left(\frac{3\pi G\hbar^2}{\langle\hat{p}_\phi\rangle^2} - \frac{4\pi^2\delta^2\ell_P^4}{\langle\hat{V}\rangle^2} \right) \frac{\langle\hat{V}\rangle^2}{(\Delta V)^2} \quad (72)$$

$$\frac{\Delta(Vp_\phi)}{\langle\hat{V}\rangle\langle\hat{p}_\phi\rangle} = \frac{(\Delta V)^2}{\langle\hat{V}\rangle^2}. \quad (73)$$

Thus,

$$\rho_{\text{eff}} = \frac{\langle\hat{\rho}\rangle}{1 - 4\pi^2\frac{\delta^2\ell_P^4}{(\Delta V)^2} + \frac{3\pi G\hbar^2}{\langle\hat{p}_\phi\rangle^2}\frac{\langle\hat{V}\rangle^2}{(\Delta V)^2} + \dots} = \frac{\langle\hat{\rho}\rangle}{1 - \epsilon\left(\frac{\rho_{\text{QG}}}{\rho_{\text{eff}}} - 1\right)} \quad (74)$$

for such a state. This equation can be solved for ρ_{eff} and implies $\rho_{\text{eff}}(1+\epsilon) = \langle\hat{\rho}\rangle + \epsilon\rho_{\text{QG}}$. If $\langle\hat{\rho}\rangle^{\text{max}} = \rho_{\text{QG}}$, $\rho_{\text{eff}}^{\text{max}} = \rho_{\text{QG}}$. If $\langle\hat{\rho}\rangle^{\text{max}} = \rho_{\text{QG}}(1+\epsilon)$, $\rho_{\text{eff}}^{\text{max}} = \rho_{\text{QG}}(1+2\epsilon)/(1+\epsilon) \sim \rho_{\text{QG}}(1+\epsilon)$. With correlations, we obtain

$$\rho_{\text{eff}} = \frac{\langle\hat{\rho}\rangle}{1 - \epsilon(1 + 4\kappa^2/\hbar^2)(\rho_{\text{QG}}/\rho_{\text{eff}} - 1) - 2\Delta(VP)/\langle\hat{V}\rangle\langle\hat{P}\rangle} \quad (75)$$

If we assume $\rho^{\text{max}} = \rho_{\text{QG}}$, $\rho_{\text{eff}}^{\text{max}} = \rho_{\text{QG}}/(1 - 2(1 + \epsilon(1 + 4\kappa^2/\hbar^2))\Delta(VP)/\langle\hat{V}\rangle\langle\hat{P}\rangle)$ is not restricted to be less than ρ_{QG} .

For a Gaussian in the scalar, the moments already computed give us

$$\frac{(\Delta V)^2}{\langle\hat{V}\rangle^2} = e^{1/\sigma^2} - 1 \quad (76)$$

$$\frac{\Delta(p_\phi V)}{\langle\hat{p}_\phi\rangle\langle\hat{V}\rangle} = e^{3/2\sigma^2}(e^{1/\sigma^2} - 1) \quad (77)$$

$$\frac{(\Delta p_\phi)^2}{\langle\hat{p}_\phi\rangle^2} = 4\left(1 + \frac{4}{\sigma^2}\right)e^{3/\sigma^2} - 2e^{1/\sigma^2} + 1 + \frac{36\pi G\hbar^2}{\langle\hat{p}_\phi\rangle^2}\left(\frac{\sigma^2}{4} + 1\right)e^{3/\sigma^2}. \quad (78)$$

The first relation can be inverted for

$$\sigma = \frac{1}{\sqrt{\log(1 + (\Delta V/\langle\hat{V}\rangle)^2)}}. \quad (79)$$

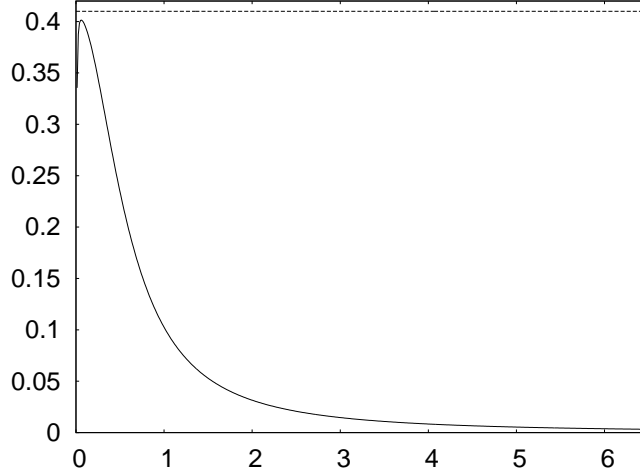


Figure 5: The effective density (80) (for $\kappa = 0$) as a function of $\Delta V / \langle \hat{V} \rangle$, assuming $\langle \hat{\rho} \rangle^{\max} = \rho_{\text{QG}}$. This plot qualitatively agrees with Fig. 20 of [13]. The quantitative difference can be explained well by the fact that we take volume fluctuations and the effective density at the same time, while [13] refers to initial volume fluctuations. Moreover, $\langle \hat{\rho} \rangle^{\max}$ may differ from ρ_{QG} in a way depending on $\Delta V / \langle \hat{V} \rangle$. The features visible in this plot are independent of $\langle \hat{p}_\phi \rangle$; see Fig. 6 for the $\langle \hat{p}_\phi \rangle$ -dependence with small $\Delta V / \langle \hat{V} \rangle$.

The final expression for ρ_{eff} in terms of $\langle \hat{\rho} \rangle$ is lengthy. We do not write it here because we have to be careful with our approximate integrals for large relative moments.

We can compute $\Delta(p_\lambda Q)$ more easily by using the \hat{p}_λ -operator, which gives us $\langle \hat{Q} \hat{p}_\lambda \rangle = \langle \hat{Q} \rangle (\frac{1}{2} i \hbar + \kappa + \bar{p}_\lambda)$, and then $\Delta(p_\lambda Q) = \text{Re} \langle \hat{Q} \hat{p}_\lambda \rangle - \langle \hat{Q} \rangle \langle \hat{p}_\lambda \rangle = \kappa$. With our previous result for Δp_λ , we have

$$\rho_{\text{eff}} = \frac{\langle \hat{\rho} \rangle}{1 + \frac{3\pi G \hbar^2}{\langle \hat{p}_\phi \rangle^2} \left(1 + 4 \frac{\kappa^2}{\hbar^2}\right) \frac{1}{\log(1 + (\Delta V)^2 / \langle \hat{V} \rangle^2)} + 3 \frac{(\Delta V)^2}{\langle \hat{V} \rangle^2} - 4 \frac{\sqrt{3\pi G \hbar^2}}{\langle \hat{p}_\phi \rangle} \frac{\kappa}{\hbar}}. \quad (80)$$

Assuming a maximum $\langle \hat{\rho} \rangle$ given by ρ_{QG} , (80) as a function of $\Delta V / \langle \hat{V} \rangle$ is shown in Fig. 5 for $\kappa = 0$ and in Fig. 6 for different values of κ . For large κ / \hbar , the maximum effective density depends on κ and $\langle \hat{p}_\phi \rangle$ mainly through the combination $\kappa / \langle \hat{p}_\phi \rangle$.

4 Conclusions

We have provided several applications of effective equations and constraints in quantum cosmology, focusing on background properties that are important for instabilities of initial-value problems in Euclidean regimes and on relations between moments that affect density bounds. The latter results provide fruitful comparisons with recent numerical evolutions of wave functions [13], showing the agreement for effective equations that include moment

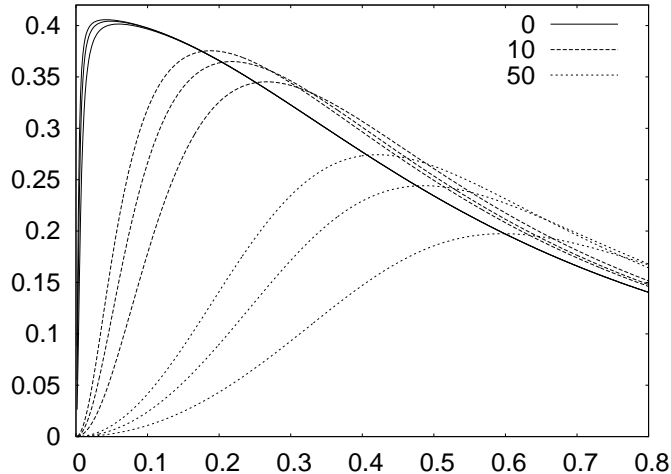


Figure 6: The effective density (80) as a function of $\Delta V/\langle\hat{V}\rangle$, assuming $\langle\hat{\rho}\rangle^{\max} = \rho_{\text{QG}}$. The maximum density obtained decreases for growing covariance. For each of the three displayed values of κ (in units with $\hbar = 1$), three curves for $\langle\hat{p}_\phi\rangle \in \{500, 750, 1000\}$ are shown. (Rather extreme values have been chosen for κ/\hbar in order to bring out the dependence on this value more clearly. For $\kappa/\hbar \sim O(1)$, the effective density does not vary much with κ/\hbar .)

terms. While [13] compared numerical results only with zeroth-order effective equations without moment terms, finding several disagreements, our application of existing effective methods show that moment-dependent corrections capture the evolution of wave functions to an excellent degree. In particular, the relations between moments derived here show that properties of physical states can be computed reliably by effective methods without having to enter technical intricacies usually associated with physical Hilbert spaces.

This conclusion has several implications for the interpretation of quantum cosmology at high density. For some time, a universal effective equation of the form (2) has been claimed to capture the evolution of a significant class of states and matter models in loop quantum cosmology. The combined results of effective equations, accumulated over several years, and recent numerical simulations shows that the equation is unreliable when moments become large and states are no longer sharply peaked. For small volume fluctuations in a Gaussian (and correspondingly large momentum fluctuations) the correction term has been derived in [3] and is one of the terms used here to show agreement with numerical simulations. For large volume fluctuations, deviations from the maximum density predicted by (2) can be explained by effective equations as well, but since their validity to second order in moments is no longer clear, the effect was brought out clearly only by the numerical simulations of [13]. Nevertheless, even for such large volume fluctuations there is, rather surprisingly, good agreement.

Effective equations and their implications are therefore reliable. One of these implica-

tions at a general level is the fact that evolution and physical properties at high density depend sensitively on the initial quantum state used, in a way that is difficult to control in quantum cosmology. The examples of states used in [13] and here make this clear, even though these states are rather limited as well. Both classes of states are Gaussian, one in the geometrical variables (Q, P) and one in the scalar pair (ϕ, p_ϕ) , and therefore much restricted even compared with a general class of semiclassical states. Nevertheless, even these restricted classes of states show marked differences for large volume fluctuations, with only small effects on the maximum density for (Q, P) -Gaussians and a strong suppression of the maximum density for (ϕ, p_ϕ) -Gaussians. One might argue that large relative volume fluctuations should not occur for a good universe model if they refer to a semiclassical initial state at low curvature (as in [13]). However, in the free, massless model there is not much quantum back-reaction, and by assuming a sharply-peaked initial state one implicitly assumes a sharply-peaked state at high density. In more-general models, relative volume fluctuations can easily grow, so that states with large relative fluctuations should indeed be considered for a generic quantum phase. Then, there is a strong sensitivity on the precise state used.

This result highlights the fact that loop quantum cosmology at large density cannot be used for reliable predictions, unless one obtains a much better understanding of relevant quantum states and possible conditions one can impose on them independently of the constraints. (The authors of [13] do not arrive at the same conclusion. Moreover, by referring to the different state choices as different “methods” of implementing initial states numerically, they hide the fact that different initial states imply different physics, and ultimately different predictions.)

We finally highlight a small but important result which has not played a large role in our considerations so far: As shown by Eq. (49), for some states the fluctuation energy may cancel completely the modification of the classical Friedmann equation that results from holonomy effects. Although this is only one example, it shows that moment terms in effective equations can easily be of the same order as holonomy corrections. Fluctuation energies considered here or, more importantly, quantum back-reaction terms in non-harmonic cosmological models with a massive or self-interacting scalar, are therefore crucial for the task of evaluating the reliability of scenarios based on holonomy effects. (This result agrees with the expectation that higher-curvature corrections generically appear in effective actions of gravity: Higher time derivatives in the corresponding effective equations result from quantum back-reaction of moments [38]. Moment terms should then be of the same order $O(\ell_P^2 \mathcal{H}^2)$ as higher-curvature corrections, which is the same order as holonomy modifications obtained by expanding the sine function in (31).) Unfortunately, not much is known about the generic behavior of quantum back-reaction in (loop) quantum cosmology. The good agreement of effective and numerical calculations confirmed in this article will hopefully lead to a more-complete understanding.

Acknowledgements

The author thanks Jaume Garriga for discussions, pointing out the important question of quantitative aspects of instabilities in Euclidean regimes. This work was supported in part by NSF grant PHY-1307408.

A Kinematical and physical moments

If we solve (55) and (56) for $\Delta(p_\lambda Q)$ and $\Delta(p_\lambda \sin(\delta P))$, respectively, we obtain complex values

$$\begin{aligned}\delta\Delta(p_\lambda Q) &= \langle \widehat{\sin(\delta P)} \rangle \Delta(Q^2) + \langle \hat{Q} \rangle \Delta(Q \sin(\delta P)) + \frac{1}{2}i\hbar\delta\langle \hat{Q} \rangle \langle \widehat{\cos(\delta P)} \rangle \\ \delta\Delta(p_\lambda \sin(\delta P)) &= \langle \widehat{\sin(\delta P)} \rangle \Delta(Q \sin(\delta P)) + \langle \hat{Q} \rangle \Delta(\sin^2(\delta P)) - \frac{1}{2}i\hbar\delta\langle \hat{Q} \rangle \langle \widehat{\cos(\delta P)} \rangle \langle \widehat{\sin(\delta P)} \rangle.\end{aligned}\tag{81}$$

(As before, we have used $\delta\langle \hat{p}_\lambda \rangle = \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle$ in coefficients of the moments, which is valid to the order considered here since squared relative moments are then small compared to the relative moments.) The imaginary terms cancel in the combination (57) which was of interest earlier on in this article, but it is still important and instructive to comment on the complex-valuedness of some moments. This feature is related to the complex nature of time expectation values in deparameterized quantum systems, noticed in [39, 40] and evaluated in a cosmological model in [41]. We will first discuss complex moments and their physical role in detail, and then apply the notion of complex time to the models studied here.

A.1 Physical states in effective constrained systems

The moments appearing in (81) involve all phase-space variables (except λ) of the original system with degrees of freedom (Q, P) and (λ, p_λ) . These are independent variables only before constraints are solved. Their quantum moments can be computed only in a kinematical Hilbert space of states that do not solve the constraints. Since moments refer to symmetric orderings of the operators involved, they must take real values when computed in the kinematical Hilbert space.

In (81), we have solved some of the effective constraints and therefore left the kinematical arena. When all constraints are imposed at the quantum level, we have moments of physical states in which some of the kinematical degrees of freedom have been removed. We can no longer consider (Q, P) and (λ, p_λ) as independent, and their expectation values and moments are related according to the effective constraints. This observation already helps to explain why imaginary contributions may occur in solutions for some of these moments: While \hat{p}_λ and \hat{Q} quantize independent degrees of freedom and commute with each other as operators on the kinematical Hilbert space, they are related and may be non-commuting on the physical Hilbert space. (Indeed, in the present example, $\hat{p}_\lambda\psi = \delta^{-1}Q\widehat{\sin(\delta P)}\psi$ on physical states.)

A.1.1 Physical moments

Transitioning from the kinematical to a physical Hilbert space is usually a complicated procedure in canonical quantum gravity and cosmology, and indeed presents one of the crucial problems to be faced. One can easily derive physical Hilbert spaces in deparameterizable systems, forming by far the largest class of models studied in this context. However, the special nature of deparameterizable systems, requiring the existence of a phase-space variable without turning points where the momentum becomes zero, makes it doubtful that results relying on deparameterizability are robust. One of the advantages of effective constraints is that they can be applied consistently to systems with local internal times at the quantum level.

Effective methods allow one to compute properties of quantum states without having to work with wave functions and explicit integral representations of inner products in Hilbert spaces. Instead, states are expressed in terms of the expectation-value functional, or the set of expectation values and moments of basic operators. As successfully used in algebraic quantum field theory [42], for instance, a state is a positive linear functional of norm one on the $*$ -algebra generated by basic operators. If one uses a Hilbert space, the $*$ -relation is turned into adjointness relations of operators. The positive linear functional applied to an element A of the $*$ -algebra is then the expectation value of a given wave function assigned to A , computed using the inner product of the Hilbert space. It turns out that many questions of interest do not require much of the structure of a Hilbert space but rather refer to general properties of states as positive linear functionals. These are exactly the properties that can be computed using canonical effective methods. (Properties that are difficult to express in this way refer to probabilities of individual measurements. Such questions rarely play a role in quantum cosmology.)

Physical normalization, in the absence of an explicit Hilbert space, is imposed by requiring all observables — expectation values and moments — to respect the $*$ -relations of the $*$ -algebra. For the usual canonical basic operators generating a $*$ -algebra, this means that all expectation values and moments must be real. This simple condition is sufficient to replace complicated constructions of integral representations of physical inner products. (Positivity of the linear functional of a state is reflected in inequalities to be satisfied by physical moments, most importantly uncertainty relations.) The general notion of states as positive linear functionals also makes it possible to formulate a unified treatment of kinematical and physical moments as used here. Both types of moments are defined on the same $*$ -algebra, but physical moments are restricted by (i) reality conditions that follow from the $*$ -relation and (ii) by effective constraints derived from constraint operators. Even when it is not possible to find a physical Hilbert space as a subset of the kinematical Hilbert space, kinematical and physical moments can be treated on the same footing. The remainder of this appendix provides new examples for this scheme.

A.1.2 Casimir constraints

Casimir constraints are special versions of first-class constraints which do not generate a gauge flow (which is possible for first-class constraints on non-symplectic spaces). They lead to restrictions of the moments, but no flow need be factored out. Unrestricted moments are therefore automatically Dirac observables.

The condition (52) provides an example for Casimir constraints. It implies an effective constraint

$$\langle \hat{T} \rangle = \langle \widehat{\sin(\delta P)} \rangle^2 + \langle \widehat{\cos(\delta P)} \rangle^2 + \Delta(\sin^2(\delta P)) + \Delta(\cos^2(\delta P)) - 1 = 0$$

as well as higher-order constraints T_{pol} . We will make use only of

$$\begin{aligned} T_{\sin(\delta P)} &= 2\langle \widehat{\sin(\delta P)} \rangle \Delta(\sin^2(\delta P) + 2\langle \widehat{\cos(\delta P)} \rangle \Delta(\sin(\delta P) \cos(\delta P))) = 0 \\ T_{\cos(\delta P)} &= 2\langle \widehat{\sin(\delta P)} \rangle \Delta(\sin(\delta P) \cos(\delta P)) + 2\langle \widehat{\cos(\delta P)} \rangle \Delta(\cos^2(\delta P)). \end{aligned}$$

We can eliminate the two moments involving $\cos(\delta P)$:

$$\begin{aligned} \Delta(\sin(\delta P) \cos(\delta P)) &= \frac{\langle \widehat{\sin(\delta P)} \rangle}{\langle \widehat{\cos(\delta P)} \rangle} \Delta(\sin^2(\delta P)) \\ \Delta(\cos^2(\delta P)) &= \frac{\langle \widehat{\sin(\delta P)} \rangle^2}{\langle \widehat{\cos(\delta P)} \rangle^2} \Delta(\sin^2(\delta P)). \end{aligned}$$

The latter allows us to write $\langle \hat{T} \rangle = 0$ as

$$\langle \widehat{\sin(\delta P)} \rangle^2 + \langle \widehat{\cos(\delta P)} \rangle^2 = \frac{1}{1 + \langle \widehat{\cos(\delta P)} \rangle^{-2} \Delta(\sin^2(\delta P))}. \quad (82)$$

A.2 Complex moments

The moment $\Delta(p_\lambda Q)$ is initially defined as a kinematical moment, in which \hat{p}_λ and \hat{Q} need not be ordered symmetrically in an explicit way because these are independent and commuting operators. Once we transition to physical states by solving effective constraints, we expect the ordering to become important because $Q \widehat{\sin(\delta P)}$ does not commute with \hat{Q} . We start with

$$\Delta(Q p_\lambda) = \langle \hat{Q} \hat{p}_\lambda \rangle - \langle \hat{Q} \rangle \langle \hat{p}_\lambda \rangle$$

as a kinematical moment, which becomes

$$\Delta(Q p_\lambda) = \frac{1}{2} \langle \hat{Q} \hat{p}_\lambda + \hat{p}_\lambda \hat{Q} \rangle - \langle \hat{Q} \rangle \langle \hat{p}_\lambda \rangle + \frac{1}{2} \langle [\hat{Q}, \hat{p}_\lambda] \rangle \quad (83)$$

in an explicit symmetric ordering. For physical moments involving p_λ , \hat{p}_λ must be ordered to the right so that we can substitute $\hat{p}_\lambda \psi = \delta^{-1} Q \widehat{\sin(\delta P)} \psi$ on physical states. (If \hat{p}_λ appears

on the left, one would have to use adjointness relations which depend on the Hilbert space used, kinematical or physical, and cannot be taken for granted at the effective level because $\widehat{Q \sin(\delta P)}$ is not a basic operator.) The commutator in (83) then provides the imaginary contribution found in (81).

While $\Delta(Qp_\lambda)$ as the covariance of two independent variables is no longer defined for physical states, one can interpret it as a composite moment in which \hat{p}_λ is understood as the operator $\delta^{-1} \widehat{Q \sin(\delta P)}$. There should then be a physical moment for it, which, unlike (81) must be real. A simple guess suggests that the physical moment is just the real part of (81), or

$$\Delta_{\text{phys}}(Qp_\lambda) = \langle \hat{Q} \rangle \Delta_{\text{phys}}(Q \sin(\delta P)) + \langle \widehat{\sin(\delta P)} \rangle \Delta_{\text{phys}}(Q^2). \quad (84)$$

One can confirm this guess by computing $\Delta_{\text{phys}}(Qp_\lambda)$ for states annihilated by the constraint, that is after substituting $\frac{1}{2}(\widehat{\hat{Q} \sin(\delta P)} + \widehat{\sin(\delta P) \hat{Q}})$ for $\delta \hat{p}_\lambda$ and symmetrizing \hat{Q} and \hat{p}_λ :

$$\begin{aligned} \delta \Delta_{\text{phys}}(Qp_\lambda) &= \frac{1}{2} \delta \langle \hat{Q} \hat{p}_\lambda + \hat{p}_\lambda \hat{Q} \rangle - \delta \langle \hat{Q} \rangle \langle \hat{p}_\lambda \rangle \\ &= \frac{1}{4} \langle \widehat{\hat{Q} \sin(\delta P) \hat{Q}} + \widehat{\sin(\delta P) \hat{Q}^2} + \widehat{\hat{Q}^2 \sin(\delta P)} + \widehat{\hat{Q} \sin(\delta P) \hat{Q}} \rangle \\ &\quad - \frac{1}{2} \langle \hat{Q} \rangle \langle \widehat{\hat{Q} \sin(\delta P)} + \widehat{\sin(\delta P) \hat{Q}} \rangle. \end{aligned} \quad (85)$$

The ordering obtained in this way is not Weyl, but one can rearrange so that

$$\frac{1}{4} \left(\widehat{\hat{Q} \sin(\delta P) \hat{Q}} + \widehat{\sin(\delta P) \hat{Q}^2} + \widehat{\hat{Q}^2 \sin(\delta P)} + \widehat{\hat{Q} \sin(\delta P) \hat{Q}} \right) = (\widehat{\hat{Q}^2 \sin(\delta P)})_{\text{Weyl}} - \frac{1}{12} \hbar^2 \delta^2 \widehat{\sin(\delta P)}.$$

Moreover, for any third-order moment of the form $\Delta(A^2 B)$ we have

$$\Delta(Q^2 \sin(\delta P)) = \langle (\widehat{\hat{Q}^2 \sin(\delta P)})_{\text{Weyl}} \rangle - 2 \langle \hat{Q} \rangle \Delta(Q \sin(\delta P)) - \langle \widehat{\sin(\delta P)} \rangle \Delta(Q^2) - \langle \hat{Q} \rangle^2 \langle \widehat{\sin(\delta P)} \rangle.$$

Applying this for one term in our physical moment, we obtain

$$\delta \Delta_{\text{phys}}(Qp_\lambda) = \Delta_{\text{phys}}(Q^2 \sin(\delta P)) + \langle \hat{Q} \rangle \Delta_{\text{phys}}(Q \sin(\delta P)) + \langle \widehat{\sin(\delta P)} \rangle \Delta_{\text{phys}}(Q^2) - \frac{1}{2} \hbar^2 \delta^2 \langle \widehat{\sin(\delta P)} \rangle, \quad (86)$$

which indeed agrees with the real part of (81) within the present approximation, in which the third-order moment $\Delta_{\text{phys}}(Q^2 \sin(\delta P)) = O(\hbar^{3/2})$ and the re-ordering term of order \hbar^2 are small compared with the second-order moments of order \hbar . A similar result holds for $\Delta_{\text{phys}}(p_\lambda^2)$, which can be shown to be

$$\begin{aligned} \delta^2 \Delta_{\text{phys}}(p_\lambda^2) &= \Delta_{\text{phys}}(Q^2 \sin^2(\delta P)) - \Delta_{\text{phys}}(Q \sin(\delta P))^2 \\ &\quad + \frac{1}{4} \hbar^2 \delta^2 \left(1 - \frac{1}{3} (\Delta_{\text{phys}}(\sin^2(\delta P)) + \langle \widehat{\sin(\delta P)} \rangle^2) \right) \\ &\quad + 2 \langle \hat{Q} \rangle \Delta_{\text{phys}}(Q \sin^2(\delta P)) + 2 \langle \widehat{\sin(\delta P)} \rangle \Delta_{\text{phys}}(Q^2 \sin(\delta P)) \\ &\quad + \langle \hat{Q} \rangle^2 \Delta_{\text{phys}}(\sin^2(\delta P)) + \langle \widehat{\sin(\delta P)} \rangle^2 \Delta_{\text{phys}}(Q^2) + 2 \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \Delta_{\text{phys}}(Q \sin(\delta P)) \end{aligned} \quad (87)$$

on physical states. Compared with these calculations that require explicit re-orderings, deriving moments from effective constraints is much easier.

A.3 Complex time

So far, in this appendix, we have not used deparameterization to distinguish one of the phase-space variables (or an expectation value) as time. Doing so sheds more light on the complex nature of moments, as well as the time expectation value.

A.3.1 Scalar time

If we choose λ as time, as in the main body of this article, expectation values and moments involving λ and p_λ are no longer independent of those of Q and P . Relationships for some of them are provided by effective constraints, as discussed. Other moments, especially those involving λ are not even defined for physical states when deparameterization is used, just as there is no strict time fluctuation in quantum mechanics. Moments involving only Q and P , on the other hand, are physical and related to Dirac observables of the effective constrained system, as shown in [36, 37]. Moments involving p_λ can be obtained after solving the constraint for \hat{p}_λ and substituting in the moments, as done in the preceding subsection and in Section 3.2.1 (see Eq. (44)).

Moments involving λ are not physical because they are not invariant under the gauge transformations generated by the effective constraints

$$C_\lambda = 2\delta^2\langle\hat{p}_\lambda\rangle\Delta(\lambda p_\lambda) + i\hbar\delta^2\langle\hat{p}_\lambda\rangle - 2\langle\hat{Q}\rangle\langle\widehat{\sin(\delta P)}\rangle^2\Delta(\lambda Q) - 2\langle\hat{Q}\rangle^2\langle\widehat{\sin(\delta P)}\rangle\Delta(\lambda\sin(\delta P)) \quad (88)$$

and (54), (55), (56). Following [39, 40], one can see that the conditions

$$0 = \phi_1 := \Delta(\lambda^2) \quad , \quad 0 = \phi_2 := \Delta(\lambda Q) \quad , \quad 0 = \phi_3 := \Delta(\lambda\sin(\delta P)) \quad (89)$$

are good gauge-fixing conditions for the first-order constraints C_λ , C_{p_λ} , C_Q and $C_{\sin(\delta P)}$. (Since second-order moments have a Poisson structure that is not invertible, three gauge-fixing conditions suffice for four first-class constraints. See [43] for constraints on non-symplectic spaces.) We can then immediately solve the constraint $C_\lambda = 0$ to obtain $\Delta(\lambda p_\lambda) = -\frac{1}{2}i\hbar$. (As a non-physical moment evaluated for physical states, this moment need not be real. The complex value ensures that the uncertainty relation is valid even with $\Delta\lambda = 0$.)

After imposing the gauge-fixing conditions $\phi_i = 0$, only one constraint is left to the orders considered, along with a corresponding gauge flow that amounts to evolution in internal time λ . The gauge generator consistent with the gauge fixing is a linear combination $N^\alpha C_\alpha$ of the four constraints which have not yet been solved (all but C_λ) so that $\{\phi_i, C_\alpha\}N^\alpha = 0$ for $i = 1, 2, 3$. Computing the matrix $\{\phi_i, C_\alpha\}$ and solving for the restricted components of N^α , we obtain the combination

$$N^\alpha C_\alpha = N \left(C - \frac{1}{2\langle\hat{p}_\lambda\rangle} C_{p_\lambda} - \frac{1}{2\langle\hat{Q}\rangle} C_Q - \frac{1}{2\langle\widehat{\sin(\delta P)}\rangle} C_{\sin(\delta P)} \right)$$

$$= N \left(\delta^2 \langle \hat{p}_\lambda \rangle^2 - \langle \hat{Q} \rangle^2 \langle \widehat{\sin(\delta P)} \rangle^2 - 2 \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \Delta(Q \sin(\delta P)) \right)$$

with only one free multiplier N . A convenient choice is $N = 1/(\delta \langle \hat{p}_\lambda \rangle)$, which gives us the λ -Hamiltonian

$$H_\lambda \approx \langle \hat{p}_\lambda \rangle - \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle - \Delta(Q \sin(\delta P)). \quad (90)$$

(We have used the constraint $C = 0$ and ignored products of second-order moments.)

One can easily solve some of the equations of motion to leading order, ignoring moments. For instance, we have

$$\frac{d \langle \widehat{\sin(\delta P)} \rangle}{d\lambda} = \langle \widehat{\sin(\delta P)} \rangle \langle \widehat{\cos(\delta P)} \rangle, \quad \frac{d \langle \widehat{\cos(\delta P)} \rangle}{d\lambda} = -\langle \widehat{\sin(\delta P)} \rangle^2, \quad (91)$$

so that $\langle \widehat{\sin(\delta P)} \rangle^2 + \langle \widehat{\cos(\delta P)} \rangle^2 =: c$ is conserved. (This constant equals $c = 1 - \Delta(\sin^2(\delta P)) - \Delta(\cos^2(\delta P)) \sim 1$ by the Casimir constraint.) Using c , we can decouple the two equations, and solve for

$$\langle \widehat{\cos(\delta P)} \rangle(\lambda) = \sqrt{c} \tanh(-2\sqrt{c}(\lambda - \lambda_0)). \quad (92)$$

With this solution, we obtain

$$\langle \widehat{\sin(\delta P)} \rangle(\lambda) = \frac{\sqrt{c}}{\cosh(-2\sqrt{c}(\lambda - \lambda_0))}. \quad (93)$$

We can then use the constraint $H_\lambda = 0$ to find

$$\langle \hat{Q} \rangle(\lambda) = \frac{\langle \hat{p}_\lambda \rangle}{\sqrt{c}} \cosh(-2\sqrt{c}(\lambda - \lambda_0)). \quad (94)$$

The expectation value of \hat{Q} (the volume for $x = -1/2$) is bounded from below by $\langle \hat{Q} \rangle_{\min} = \langle \hat{p}_\lambda \rangle + O(\Delta(\cdot))$. (The solution for $\langle \hat{Q} \rangle$ is exact for the harmonic ordering [3].)

A.3.2 Curvature time

Although the system is not deparameterizable by P , effective constraints can be evaluated with local internal times valid only for a finite range. To this end, we follow the same procedure as before but choose gauge-fixing conditions

$$0 = \phi_1 := \Delta(\sin^2(\delta P)) \quad , \quad 0 = \phi_2 := \Delta(\lambda \sin(\delta P)) \quad , \quad 0 = \phi_3 := \Delta(p_\lambda \sin(\delta P)). \quad (95)$$

The P -Hamiltonian which preserves the new gauge-fixing conditions is now

$$H_{\sin(\delta P)} = N \left(\delta^2 \langle \hat{p}_\lambda \rangle^2 - \langle \hat{Q} \rangle^2 \langle \widehat{\sin(\delta P)} \rangle^2 - i\hbar \delta \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \langle \widehat{\cos(\delta P)} \rangle \right), \quad (96)$$

whose imaginary contribution comes from the complex $\Delta(Q \sin(\delta P)) = \frac{1}{2} i\hbar \delta \langle \widehat{\cos(\delta P)} \rangle$ (a non-physical moment when P is chosen as time). The P -Hamiltonian can be real only if

the time expectation value $\langle \widehat{\sin(\delta P)} \rangle$ is complex. (The expectation value $\langle \hat{p}_\lambda \rangle$ is physical in this choice of time and must be real.) Since the imaginary contribution to $H_{\sin(\delta P)}$ is of the order of $\hbar\delta$ and therefore small, the imaginary contribution to $\langle \widehat{\sin(\delta P)} \rangle$ is small and we can expand

$$\langle \widehat{\sin(\delta P)} \rangle = \text{Re}\langle \widehat{\sin(\delta P)} \rangle + i\delta\langle \widehat{\cos(\delta P)} \rangle I \quad (97)$$

as well as

$$\langle \widehat{\cos(\delta P)} \rangle = \text{Re}\langle \widehat{\cos(\delta P)} \rangle - i\delta\langle \widehat{\sin(\delta P)} \rangle I \quad (98)$$

with I playing the role of an imaginary part of $\langle \hat{P} \rangle$. The P -Hamiltonian is then real provided that

$$\begin{aligned} \langle \widehat{\sin(\delta P)} \rangle^2 + i\hbar\delta \frac{\langle \widehat{\sin(\delta P)} \rangle \langle \widehat{\cos(\delta P)} \rangle}{\langle \hat{Q} \rangle} &\sim (\text{Re}\langle \widehat{\sin(\delta P)} \rangle)^2 \\ + 2i\delta \text{Re}\langle \widehat{\sin(\delta P)} \rangle \text{Re}\langle \widehat{\cos(\delta P)} \rangle I + i\hbar\delta \frac{\text{Re}\langle \widehat{\sin(\delta P)} \rangle \text{Re}\langle \widehat{\cos(\delta P)} \rangle}{\langle \hat{Q} \rangle} &+ O(I^2) \end{aligned}$$

has a vanishing imaginary part. Thus, $I = -\frac{1}{2}\hbar/\langle \hat{Q} \rangle$.

We finally use this example to show that relationships between moments depend on the choice of internal time, or on the deparameterization scheme and the physical Hilbert space one may construct. With the curvature parameter P chosen as time and the gauge fixing (95), the general relation

$$\delta^2 \Delta(p_\lambda^2) = \langle \hat{Q} \rangle^2 \Delta(\sin^2(\delta P)) + \langle \widehat{\sin(\delta P)} \rangle^2 \Delta(Q^2) + 2\langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \Delta(Q \sin(\delta P))$$

reduces to

$$\delta^2 \Delta(p_\lambda^2) = \langle \widehat{\sin(\delta P)} \rangle^2 \Delta(Q^2) + i\hbar\delta \langle \hat{Q} \rangle \langle \widehat{\sin(\delta P)} \rangle \langle \widehat{\cos(\delta P)} \rangle.$$

The complex contribution is no longer surprising. The real part of this equation implies

$$\frac{\Delta_{\text{phys}} p_\lambda}{\langle \hat{p}_\lambda \rangle} = \frac{\Delta_{\text{phys}} Q}{\langle \hat{Q} \rangle}$$

for all states with the present choice of internal time, in contrast to the state-dependent and more-complicated behavior seen in the main body of this paper for λ or ϕ as internal time. This result serves as a reminder that the time variable and its momentum are not defined for physical states, neither as expectation values nor in moments. Moments of the momentum can be defined only indirectly upon using the constraint.

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